

Scattering Theory for the matrix Schrödinger operator on the half line with general boundary conditions ^{*}

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Abstract

We study the stationary scattering theory for the matrix Schrödinger equation on the half line, with the most general boundary condition at the origin, and with integrable selfadjoint matrix potentials. We prove the limiting absorption principle, we construct the generalized Fourier maps, and we prove that they are partially isometric with initial space the subspace of absolute continuity of the matrix Schrödinger operator and final space $L^2((0, \infty))$. We prove the existence and the completeness of the wave operators and we establish that they are given by the stationary formulae. We also construct the spectral shift function and we give its high-energy asymptotics. Furthermore, assuming that the potential also has a finite first moment, we prove a Levinson's theorem for the spectral shift function.

1 Introduction

Let us consider the matrix Schrödinger operator on the half line

$$H_{A,B}\psi := -\psi'' + V(x)\psi, \quad x \in (0, \infty). \quad (1.1)$$

The prime denotes the derivative with respect to the spatial coordinate x . The wavefunction $\psi(x)$ will be either an $n \times n$ matrix-valued function or it will be a column vector with n components. It is known that the most general selfadjoint boundary condition at $x = 0$ for the operator (1.1) can be formulated in several equivalent way, see [1]-[8]. However, It was proved in [6]-[8] that, without losing generality, it is useful to state them in terms of constant $n \times n$ matrices A and B as follows,

$$-B^\dagger\psi(0) + A^\dagger\psi'(0) = 0, \quad (1.2)$$

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$$-B^\dagger A + A^\dagger B = 0, \quad (1.3)$$

$$A^\dagger A + B^\dagger B > 0. \quad (1.4)$$

Note that $A^\dagger B$ is selfadjoint and the selfadjoint matrix $(A^\dagger A + B^\dagger B)$ is positive.

The matrices A, B are not uniquely defined. We can multiply them on the right by an invertible matrix T without affecting (1.2), (1.3) and (1.4), and furthermore,

$$H_{AT, BT} = H_{A, B}. \quad (1.5)$$

The potential $V(x)$ is a $n \times n$ selfadjoint matrix-valued function that is integrable in $(0, \infty)$, that is to say, each entry of the matrix V is Lebesgue measurable on $(0, \infty)$ and

$$\int_0^\infty dx \|V(x)\| < +\infty. \quad (1.6)$$

Here, $\|V(x)\|$ designates the norm of $V(x)$ as an operator on \mathbf{C}^n . Of course, a matrix-valued function is integrable in $(0, \infty)$ if and only if each entry of that matrix is integrable on $(0, \infty)$.

We suppose that V is selfadjoint,

$$V(x) = V(x)^\dagger, \quad x \in \mathbf{R}^+. \quad (1.7)$$

By the dagger we designate the matrix adjoint .

There is currently a considerable interest on this problem. Matrix Schrödinger operators on the half line are important in quantum mechanical scattering of particles with internal structure, in quantum graphs and in quantum wires. See, for example, [1]- [5] and [9]- [21], and the references quoted there. The matrix Schrödinger operator on the half line (1.1) corresponds to a star graph. It describes the behavior of n connected very thin quantum wires that form a star-graph, i.e. a graph with only one vertex and a finite number of edges of infinite length. The boundary conditions (1.2), (1.3) and (1.4) impose restrictions on the value of the wave function and of its derivatives at the vertex. The problem has physical relevance to designing elementary gates in quantum computing and nanotubes for microscopic electronic devices, where, for example, strings of atoms may form a star-shaped graph. The consideration of general boundary conditions at the vertex, rather than, say, just Dirichlet boundary condition is relevant. For quantum graphs are important boundary conditions at the vertices that link the values, at the different edges, of the wave function and of the first derivatives. An important example is the Kirchoff boundary condition that amounts to the continuity of the wave function and the conservation of the current at the vertex. Actually, a quantum graph is an idealization of wires with a small cross section that meet at vertices. The quantum graph is obtained in the limit when the cross section goes to zero. The boundary condition on the graph's vertices depends in how the limit is taken.

From this point of view, it is of interest to study all the selfadjoint boundary conditions (1.2), (1.3), (1.4) as they can appear in various limit procedures.

in [6] the matrix Schrödinger equation in the half line was considered with a self-adjoint matrix potential and with the most general self-adjoint boundary condition at the origin. For matrix potentials that are integrable and have a finite first moment, it was proven that the scattering matrix is continuous at zero energy, and an explicit formula for its value at zero energy was given. Also, the small-energy asymptotics was established for the Jost matrix, its inverse, and other quantities that are important in direct and inverse scattering problems. The paper [6] is complementary to the classical monograph by Agranovich and Marchenko [22] that only considers the Dirichlet boundary condition, but where the behavior at zero energy is studied. The article [6] is also complementary to the results by Harmer, [3, 4, 5] where matrix Schrödinger operators on the half line with general boundary conditions are investigated, but the small-energy analysis is not considered.

The paper [7] considers the high-energy asymptotics for the Jost matrix, for its inverse and for the scattering matrix. Also Levinson's theorem was proven. This theorem relates the number of bound states to the change in the argument of the determinant of the scattering matrix. The article [7] complements Agranovich and Marchenko's results [22] who gave the large energy asymptotics and Levinson's theorem, but only under the Dirichlet boundary condition. The contribution [7] also complements the study [3, 4, 5] by Harmer (see also [23]), where the general selfadjoint boundary condition is considered but the large-energy asymptotics of the scattering matrix is obtained by only providing the leading term, with the remaining terms given as $o(1)$ for large energy. In [23], the leading term is given, but we also obtain the next-order term, that behaves as $1/k$ with k the square root of the energy and the large-energy asymptotics up to $O(1/k^2)$ is obtained, which is crucial in establishing the Fourier transform of several quantities that are important in the inverse scattering problem. In [8] the results of [6] are improved in the case where the potential is integrable and has a finite second moment. It is proven that the scattering matrix is differentiable at zero energy, and an explicit formula is given for its derivative at zero energy. Also, [8] improves, in the case where the second moment of the potential is finite, the small -energy asymptotics given in [6] for the Jost matrix, its inverse, and other quantities important in the direct and inverse scattering problems.

In this paper we complement the results of [6]-[8] by studying the stationary scattering theory of the matrix Schrödinger operator $H_{A,B}$ in equation (1.1), with the most general boundary condition (1.2)-(1.4) and with matrix potentials that satisfy (1.6) and (1.7).

The paper is organized as follows. In Section 2 we introduce notations and definitions that we use throughout the paper. In Section 3 we state results from [6]-[8], that we need, in the Jost solution, the regular solution, the Jost and scattering matrices and in transformations of the matrices A, B that give the boundary conditions. In Section 4 we construct a selfadjoint realization of the matrix Schrödinger operator (1.1), that we also denote by $H_{A,B}$, using

quadratic forms. In Section 5 we study the resolvent of $H_{A,B}$ and we prove the limiting absorption principle. It is customary in scattering theory to formulate the limiting absorption principle in terms of weighted L^2 spaces or of a Besov space and its dual. See for example [24]-[27]. On the contrary, since we work under the condition that the potential matrix V is only integrable, we have found it more convenient to formulate the limiting absorption principle between L^1 and L^∞ . In Section 6 we construct the generalized Fourier maps. In Section 7 we study the wave operators. Section 8 is dedicated to the scattering operator and the scattering matrix. Finally, in Section 9 the spectral shift function is constructed and a Levinson's theorem for the spectral shift function is proven.

2 Notations and definitions

We designate by \mathbf{C}^+ the upper-half complex plane, by \mathbf{R} the real axis, and we let $\overline{\mathbf{C}^+} := \mathbf{C}^+ \cup \mathbf{R}$. For any $k \in \overline{\mathbf{C}^+}$ we denote by k^* its complex conjugate. For any matrix D we designate by D^\dagger its adjoint. We denote by C a positive constant that might not take the same value when it appears in different places.

We denote by L^p , $1 \leq p \leq \infty$, the standard space $L^p((0, \infty))$ of measurable functions with values in \mathbf{C}^n , in particular, we will use L^2 instead of $L^2((0, \infty))$, for simplicity.

By H_l , $l = 1, 2$, we denote the Sobolev space of order l of all square integrable, complex valued functions with all distributional derivatives up to order l given by square integrable functions [28]. We designate by $H_{1,0}$ the completion of $C_0^\infty((0, \infty))$ in the norm of H_1 , where $C_0^\infty((0, \infty))$ is the space of all infinitely differentiable, complex valued functions with compact support. We use the notation,

$$\mathbf{H}_l := \oplus_{j=1}^n H_l, \quad l = 1, 2, \quad (2.1)$$

for the first and second Sobolev spaces of functions with values in \mathbf{C}^n .

Let $\mathbf{W}_{l,\infty}$, $l = 1, 2$ be the Sobolev space of all measurable functions on $(0, \infty)$ with values in \mathbf{C}^n that together with all its derivatives of order up to l are essentially bounded [28].

For any pair of Banach spaces X, Y we designate by $\mathcal{B}(X, Y)$ the Banach space of all bounded linear operators from X into Y . In the case where $X = Y$ we use $\mathcal{B}(X)$ instead of $\mathcal{B}(X, X)$.

For any Hilbert-Schmidt operator G we denote by $\|G\|_2$ its Hilbert-Schmidt norm and for any trace class operator G we denote by $\|G\|_1$ its trace norm and by $\text{Tr}(G)$ its trace. For any densely defined operator D in a Banach space we denote by $\rho(D)$ its resolvent set, i.e., the open set of all $z \in \mathbf{C}$ such that $D - z$ is invertible and $(D - z)^{-1}$ is bounded.

For any selfadjoint operator \mathbf{H} we denote by $\mathcal{H}_{ac}(\mathbf{H})$ its subspace of absolute continuity and by $P_{ac}(\mathbf{H})$ the projector onto $\mathcal{H}_{ac}(\mathbf{H})$.

For any pair, $\mathbf{H}_0, \mathbf{H}_1$ of selfadjoint operators in the same Hilbert space we denote the wave operators by,

$$W_{\pm}(\mathbf{H}_1, \mathbf{H}_0) := s - \lim_{t \rightarrow \pm\infty} e^{it\mathbf{H}_1} e^{-it\mathbf{H}_0} P_{ac}(\mathbf{H}_0),$$

provided that the strong limits exist. The wave operators are complete if $\text{Range}[W_{\pm}(\mathbf{H}_1, \mathbf{H}_0)] = \mathcal{H}_{ac}(\mathbf{H}_1)$. The scattering operator is defined as,

$$S(\mathbf{H}_1, \mathbf{H}_0) := (W_+(\mathbf{H}_1, \mathbf{H}_0))^* W_-(\mathbf{H}_1, \mathbf{H}_0).$$

3 Preliminary results

In this section we introduce certain results that we need. See [6, 7, 8, 22]. We always assume that V satisfies (1.6), (1.7). We first consider some $n \times n$ matrix solutions to the equation

$$-\psi'' + V(x)\psi = k^2\psi, \quad x \in (0, \infty), k \in \overline{\mathbf{C}^+}. \quad (3.1)$$

For any pair F, G of $n \times n$ matrix valued functions defined on $(0, \infty)$, we denote by,

$$[F; G] := FG' - F'G$$

the Wronskian. It follows from a direct calculation that for any two $n \times n$ solutions $\phi(k, x)$ and $\psi(k, x)$ to (3.1), each of the Wronskians $[\phi(k^*, x)^\dagger; \psi(k, x)]$ and $[\phi(-k^*, x)^\dagger; \psi(k, x)]$ is independent of x .

The Jost solution to (3.1) is the $n \times n$ matrix solution satisfying, for $k \in \overline{\mathbf{C}^+} \setminus \{0\}$, the asymptotics

$$f(k, x) = e^{ikx}[I_n + o(1/x)], \quad f'(k, x) = ik e^{ikx}[I_n + o(1/x)], \quad x \rightarrow +\infty, \quad (3.2)$$

where I_n denotes the $n \times n$ identity matrix. It is well known [6, 22], that for each fixed x , $f(k, x)$ and $f'(k, x)$ are analytic for $k \in \mathbf{C}^+$ and continuous for $k \in \overline{\mathbf{C}^+}$. It follows from (3.2) that for each fixed $k \in \mathbf{C}^+$, each of the n columns of $f(k, x)$ decays exponentially to zero as $x \rightarrow +\infty$. We have that,

$$[f(\pm k, x)^\dagger; f(\pm k, x)] = \pm 2ik I_n, \quad k \in \mathbf{R}, \quad (3.3)$$

$$[f(-k^*, x)^\dagger; f(k, x)] = 0, \quad k \in \overline{\mathbf{C}^+}. \quad (3.4)$$

The matrix Schrödinger equation (3.1) also has the $n \times n$ matrix solution $g(k, x)$ that satisfies, for each $k \in \overline{\mathbf{C}^+} \setminus \{0\}$, the following asymptotics (see page 38 of [22])

$$g(k, x) = e^{-ikx}[I_n + o(1/x)], \quad g'(k, x) = -ik e^{-ikx}(I + o(1/x)), \quad x \rightarrow \infty. \quad (3.5)$$

It is proven in [22] that $g(k, x)$ and $g'(k, x)$ are analytic in $k \in \mathbf{C}^+$ and continuous in $k \in \overline{\mathbf{C}^+} \setminus \{0\}$ for each fixed x . Equation (3.5) implies that each of the n columns of $g(k, x)$ grows exponentially as $x \rightarrow +\infty$ for each fixed $k \in \mathbf{C}^+$.

It follows from (3.2) and (3.5) that,

$$[f(-k^*, x)^\dagger; g(k, x)] = -2ik, \quad [g(-k^*, x)^\dagger; f(k, x)] = 2ik, \quad [g(-k^*, x)^\dagger; g(k, x)] = 0. \quad (3.6)$$

On page 28 of [22] it is also proven that for each $k \in \overline{\mathbf{C}^+} \setminus \{0\}$, the combined $2n$ columns of $f(k, x)$ and of $g(k, x)$ form a fundamental set of solutions to (3.1). Hence, any column-vector solution $\omega(k, x)$ to (3.1) can be written as a linear combination of them,

$$\omega(k, x) = f(k, x) \xi + g(k, x) \eta, \quad (3.7)$$

for some constant column vectors ξ and η in \mathbf{C}^n .

The regular solution $\varphi_{A,B}(k, x)$ is the $n \times n$ matrix solution to (3.1) that satisfies the initial conditions

$$\varphi_{A,B}(k, 0) = A, \quad \varphi'_{A,B}(k, 0) = B, \quad (3.8)$$

where A and B are the matrices appearing in (1.2), (1.3), (1.4). It is known that [6], for each fixed $x \in \mathbf{R}^+$, $\varphi(k, x)$ is entire in k in the complex plane \mathbf{C} . As k^2 appears in (3.1) and the initial values given in (3.8) are independent of k ,

$$\varphi(-k, x) = \varphi(k, x), \quad k \in \mathbf{C}, \quad x \in (0, \infty). \quad (3.9)$$

The Jost matrix $J(k)$ is defined as follows,

$$J_{A,B}(k) := [f(-k^*, x)^\dagger; \varphi_{A,B}(k, x)], \quad k \in \overline{\mathbf{C}^+}. \quad (3.10)$$

Evaluating the Wronskian at $x = 0$ and using (3.8) we obtain that,

$$J_{A,B}(k) = f(-k^*, 0)^\dagger B - f'(-k^*, 0)^\dagger A, \quad k \in \overline{\mathbf{C}^+}. \quad (3.11)$$

Note that $J(k)$ is well defined for $\overline{\mathbf{C}^+}$ because $f(-k^*, 0)^\dagger$ and $f'(-k^*, 0)^\dagger$ are analytic in $k \in \mathbf{C}^+$ and continuous in $k \in \overline{\mathbf{C}^+}$. Furthermore [6], $J(k)$ is invertible for $k \in \mathbf{R} \setminus 0$ and $J(k)^{-1}$ is continuous for $k \in \mathbf{R} \setminus 0$.

The regular solution can be expressed in terms of the Jost solution and the Jost matrix as follows (see equation (3.5) of [7]),

$$\varphi_{A,B}(k, x) = \frac{1}{2ik} f(k, x) J_{A,B}(-k) - \frac{1}{2ik} f(-k, x) J_{A,B}(k), \quad k \in \mathbf{R} \setminus \{0\}. \quad (3.12)$$

Let us define the physical solution $\psi_{A,B}(k, x)$ as follows,

$$\psi_{A,B}(k, x) := -ik \varphi_{A,B}(k, x) J_{A,B}^{-1}(k). \quad (3.13)$$

Note that there is a difference by a factor of 2 with the physical solutions defined in equation (3.7) of [7]. The scattering matrix is defined as,

$$S_{A,B}(k) := -J_{A,B}(-k) J_{A,B}(k)^{-1}, \quad k \in \mathbf{R} \setminus 0. \quad (3.14)$$

Then, the scattering matrix $S_{A,B}(k)$ is unitary for $k \in \mathbf{R} \setminus 0$ and it satisfies,

$$S(-k) = S(k)^{-1} = S(k)^\dagger, \quad k \in \mathbf{R} \setminus 0. \quad (3.15)$$

The physical solution can be written in terms of the Jost solution and the scattering matrix as follows (see equation (3.10) of [7]),

$$\psi_{A,B}(k, x) := \frac{1}{2} f(-k, x) + \frac{1}{2} f(k, x) S_{A,B}(k), \quad k \in \mathbf{R} \setminus 0. \quad (3.16)$$

Note that as the physical solution (3.13) differs by a factor of 2 with the physical solutions defined in equation (3.7) of [7], equation (3.16) differs by a factor of 1/2 with equation (3.10) of [7]. Equations (3.12) and (3.16) hold under the assumption that V is integrable. The condition that V also has a finite first moment is only needed in [7] in order that (3.16) also holds for $k = 0$.

Let A, B be the matrices that appear in the definition of the boundary conditions in equations (1.2), (1.3) and (1.4). In Proposition 4.1 of [7] it is proven that if A, B are multiplied on the right by an invertible matrix T , and if V is unchanged, the regular solution, the Jost matrix and the scattering matrix change as follows,

$$\varphi_{AT,BT}(k, x) = \varphi_{A,B}(k, x) T, \quad k \in \mathbf{C}, \quad (3.17)$$

$$J_{AT,BT}(k) = J_{A,B}(k, x) T, \quad k \in \overline{\mathbf{C}^+}, \quad (3.18)$$

$$S_{AT,BT}(k) = S_{A,B}(k), \quad k \in \mathbf{R} \setminus 0. \quad (3.19)$$

Furthermore, it is also proven in Proposition 4.1 of [7] (with M, M^\dagger there, replaced, respectively, by M^\dagger, M) that under the unitary transformation $V \mapsto MVM^\dagger$, with a unitary matrix M , and the combination of three consecutive transformation $(A, B) \mapsto (MAT_1M^\dagger T_2, MBT_1M^\dagger T_2)$, first by a right multiplication by an invertible matrix T_1 , then by the unitary transformation with M , followed by a right multiplication by an invertible matrix T_2 , we have that

$$f_{MVM^\dagger}(k, x) = M f(k, x) M^\dagger, \quad k \in \overline{\mathbf{C}^+}, \quad (3.20)$$

$$\varphi_{MVM^\dagger, MAT_1M^\dagger T_2, MBT_1M^\dagger T_2}(k, x) = M \varphi_{V,A,B}(k, x) T_1 M^\dagger T_2, \quad k \in \mathbf{C}, \quad (3.21)$$

$$J_{MVM^\dagger, MAT_1M^\dagger T_2, MBT_1M^\dagger T_2}(k, x) = M J_{V,A,B}(k, x) T_1 M^\dagger T_2, \quad k \in \overline{\mathbf{C}^+}, \quad (3.22)$$

$$S_{MVM^\dagger, MAT_1M^\dagger T_2, MBT_1M^\dagger T_2} = M S_{V,A,B} M^\dagger, \quad k \in \mathbf{R} \setminus 0. \quad (3.23)$$

In (3.20)- (3.23) we made explicit, for clarity, the dependence in V of the Jost solution, the regular solution, the Jost matrix and the scattering matrix.

Furthermore, we have that,

$$H_{MVM^\dagger, MAT_1M^\dagger T_2, MBT_1M^\dagger T_2} = M H_{V,A,B} M^\dagger, \quad (3.24)$$

where we also made explicit the dependence in V of the matrix Schrödinger operator (1.1).

The transformation $V \mapsto V$ and $(A, B) \mapsto (AT, BT)$ with an invertible matrix T is just a change of parametrization in the boundary conditions (1.2), (1.3) and (1.4). On the contrary, the unitary transformation $V \mapsto MVM^\dagger$ and $(A, B) \mapsto (MAM^\dagger, MBM^\dagger)$ with a unitary matrix M is a change of representation in quantum mechanical sense.

It is useful to consider the case where the matrices A, B are diagonal. This is motivated by the general selfadjoint boundary condition [29, 30, 31] in the scalar case, i.e. when $n = 1$. We denote this special pair of diagonal matrices by \tilde{A} and \tilde{B} , where

$$\tilde{A} := -\text{diag}\{\sin \theta_1, \dots, \sin \theta_n\}, \quad \tilde{B} := \text{diag}\{\cos \theta_1, \dots, \cos \theta_n\}. \quad (3.25)$$

In this case the boundary conditions (1.2) are,

$$\cos \theta_j \psi_j(0) + \sin \theta_j \psi'_j(0) = 0, \quad j = 1, 2, \dots, n. \quad (3.26)$$

The real parameters θ_j take values in the interval $(0, \pi]$. The case $\theta_j = \pi/2$ corresponds to the Neumann boundary condition, case $\theta_j = \pi$ corresponds to the Dirichlet boundary condition, and the case where $\theta_j \neq \pi/2, \pi$ corresponds to mixed boundary conditions. We suppose that there are n_N values with $\theta_j = \pi/2$ and n_D values with $\theta_j = \pi$, and hence there are n_M remaining values, with $n_M := n - n_N - n_D$, such that the corresponding θ_j -values lie in the interval $(0, \pi/2)$ or $(\pi/2, \pi)$. We allow for the special cases where any of n_N , n_D , and n_M may be zero or n . The subscripts N, D, and M refer, respectively, to Neumann, Dirichlet or mixed boundary conditions. We order the θ_j -values in (3.25) so that the first n_M values of θ_j correspond to the mixed boundary conditions, the next n_D values correspond to the Dirichlet boundary conditions, and the remaining n_N values correspond to the Neumann boundary conditions.

Note that \tilde{A}, \tilde{B} satisfy (1.2), (1.3), (1.4) with \tilde{A}, \tilde{B} instead of A, B there.

In Proposition 4.3 of [7] it is proven that for any pair of matrices (A, B) that satisfy (1.2)-(1.4) there is a pair of diagonal matrices (\tilde{A}, \tilde{B}) as in (3.25), a unitary matrix M and two invertible matrices T_1, T_2 such that,

$$A = M \tilde{A} T_2 M^\dagger T_1, \quad B = M \tilde{B} T_2 M^\dagger T_1. \quad (3.27)$$

Note that T_1, T_2 in (3.27) correspond, respectively to T_1^{-1}, T_2^{-1} in Proposition 4.3 of [7].

For $V \equiv 0$, we have that (see Section V of [7]),

$$J_{0,A,B}(k) = B - ikA, \quad S_{0,A,B}(k) = -(B + ikA)(B - ikA)^{-1}. \quad (3.28)$$

Furthermore, in the parametrization of the boundary conditions with \tilde{A} and \tilde{B} these matrices are diagonal,

$$J_{0,\tilde{A},\tilde{B}}(k) = \tilde{B} - ik\tilde{A} = \text{diag}\{\cos\theta_1 + ik\sin\theta_1, \dots, \cos\theta_{n_M} + ik\sin\theta_{n_M}, -I_{n_D}, ikI_{n_N}\}, \quad (3.29)$$

$$J_{0,\tilde{A},\tilde{B}}(k)^{-1} = \text{diag}\left\{\frac{1}{\cos\theta_1 + ik\sin\theta_1}, \dots, \frac{1}{\cos\theta_{n_M} + ik\sin\theta_{n_M}}, -I_{n_D}, \frac{1}{ik}I_{n_N}\right\}, \quad (3.30)$$

$$S_{0,\tilde{A},\tilde{B}}(k) = \text{diag}\left\{\frac{-\cos\theta_1 + ik\sin\theta_1}{\cos\theta_1 + ik\sin\theta_1}, \dots, \frac{-\cos\theta_{n_M} + ik\sin\theta_{n_M}}{\cos\theta_{n_M} + ik\sin\theta_{n_M}}, -I_{n_D}, I_{n_N}\right\}. \quad (3.31)$$

Moreover,

$$\varphi_{0,\tilde{A},\tilde{B}} = \text{diag}\{\varphi_{0,\tilde{A},\tilde{B},1}, \varphi_{0,\tilde{A},\tilde{B},2}, \dots, \varphi_{0,\tilde{A},\tilde{B},n}\}, \quad (3.32)$$

where,

$$\varphi_{0,\tilde{A},\tilde{B},j} = \begin{cases} -\frac{1}{k} \sin kx, & \text{if } \theta_j = \pi, \\ -\cos kx, & \text{if } \theta_j = \pi/2, \\ \frac{1}{k} \cos\theta_j \sin kx - \sin\theta_j \cos kx, & \text{if } \theta_j \neq \pi, \pi/2. \end{cases} \quad (3.33)$$

In Theorem 7.6 of [7] it proven that (note the slight change of notation with respect to Theorem 7.6 of [7])

$$S_{A,B}(k) = S_{A,B}(\infty) + \frac{G(k)}{ik} + O(1/k^2), \quad k \rightarrow \pm\infty, \quad (3.34)$$

where

$$S_{A,B}(\infty) := MZ_0M^\dagger, \quad (3.35)$$

$$G(k) := -2MZ_1M^\dagger + Q_1S_{A,B}(\infty) + S_{A,B}(\infty)Q_1 + S_{A,B}(\infty)Q_2(k)S_{A,B}(\infty) + Q_2(-k), \quad (3.36)$$

with M the unitary matrix that appears in (3.27),

$$Z_0 := \text{diag}\{I_{n_M}, -I_{n_D}, I_{n_N}\}. \quad (3.37)$$

$$Z_1 := \text{diag}\{\cot\theta_1, \dots, \cot\theta_{n_M}, 0_{n_D}, 0_{n_N}\}. \quad (3.38)$$

For the definition of $\theta_1, \dots, \theta_{n_M}, n_D, n_N$ see (3.25), the text below this equation and (3.27). Furthermore, Q_1 and $Q_2(k)$ are the following matrices,

$$Q_1 := \frac{1}{2} \int_0^\infty dy V(y), \quad Q_2(k) := \frac{1}{2} \int_0^\infty dy e^{2iky} V(y).$$

4 The Hamiltonian

4.1 The case of zero potential

We consider first the case where the potential V is zero. We denote by $H_{0,A,B}$ the self-adjoint realization of $-\frac{d^2}{dx^2}$ with the boundary condition (1.2), namely

$$H_{0,A,B}\psi = -\frac{d^2}{dx^2}\psi, \quad \psi \in D(H_{0,A,B}), \quad (4.1)$$

where

$$D(H_{0,A,B}) := \{\psi \in \mathbf{H}_2 : -B^\dagger \psi(0) + A^\dagger \psi'(0) = 0\}. \quad (4.2)$$

Note that $H_{0,AT,BT} = H_{0,A,B}$ for all invertible matrices T . Recall that in the particular case of the diagonal matrices \tilde{A}, \tilde{B} (3.25) the boundary conditions (1.2) are given by (3.26). These equations can be written as,

$$\psi'(0) = -\cot \theta_j \psi_j(0), \text{ if } \theta_j \neq \pi, \text{ and } \quad \psi_j(0) = 0, \text{ if } \theta_j = \pi. \quad (4.3)$$

Let us construct the quadratic form associated to $H_{0,\tilde{A},\tilde{B}}$. We denote,

$$H_{1,j} := H_{1,0}, \text{ if } \theta_j = \pi, \text{ and } \quad H_{1,j} := H_1, \text{ if } \theta_j \neq \pi. \quad (4.4)$$

We designate,

$$\mathbf{H}_{1,\tilde{A},\tilde{B}} := \oplus_{j=1}^n H_{1,j}. \quad (4.5)$$

We define the quadratic form with domain $\mathbf{H}_{1,\tilde{A},\tilde{B}}$,

$$h_{0,\tilde{A},\tilde{B}}(\varphi, \psi) := (\varphi', \psi') - \sum_{j=1}^n \widehat{\cot} \theta_j \varphi_j(0) \overline{\psi_j(0)}, \quad (4.6)$$

where $\widehat{\cot} \theta_j = 0$ if $\theta_j = \pi/2$, or $\theta_j = \pi$, and $\widehat{\cot} \theta_j = \cot \theta_j$ if $\theta_j \neq \pi/2, \pi$.

Since, for any $\varepsilon > 0$ there is a constant K_ε such that,

$$|\psi(0)| \leq \varepsilon \|\psi\|_{\mathbf{H}_1} + K_\varepsilon \|\psi\|_{L^2}, \quad (4.7)$$

the symmetric form $h_{0,\tilde{A},\tilde{B}}$ is closed and bounded below. It follows from Theorems 2.1 and 2.6 in chapter 6 of [32] that $H_{0,\tilde{A},\tilde{B}}$ is the selfadjoint bounded below operator associated to the quadratic form $h_{0,\tilde{A},\tilde{B}}$.

We define the diagonal matrix

$$\Theta := \text{Diag} \{\widehat{\cot} \theta_1, \widehat{\cot} \theta_2, \dots, \widehat{\cot} \theta_n\}. \quad (4.8)$$

Then, by (3.24), (3.27), (4.6) the quadratic form associated to $H_{0,A,B}$ is given by,

$$h_{0,A,B}(\varphi, \psi) := (\varphi', \psi') - \sum_{j=1}^n \langle M\Theta M^\dagger \varphi(0), \psi(0) \rangle, \quad (4.9)$$

where by $\langle \cdot, \cdot \rangle$ we denote the scalar product in \mathbf{C}^n , and the domain of $h_{0,A,B}$ is given by

$$D(h_{0,A,B}) = \mathbf{H}_{1,A,B} \quad \text{where } \mathbf{H}_{1,A,B} := M\mathbf{H}_{1,\tilde{A},\tilde{B}} \subset \mathbf{H}_1. \quad (4.10)$$

4.2 The case of integrable potential

Suppose that V satisfies (1.6), (1.7). Let us define the following quadratic form,

$$h_{A,B}(\varphi, \psi) := h_{0,A,B}(\varphi, \psi) + (V\varphi, \psi), \quad D(h_{A,B}) = \mathbf{H}_{1,A,B}. \quad (4.11)$$

By (4.7), for any $\varepsilon > 0$ there is a constant K_ε such that,

$$|(V\varphi, \varphi)| \leq \varepsilon \|\varphi\|_{\mathbf{H}_1}^2 + K_\varepsilon \|\varphi\|_{L^2}^2.$$

Hence, the symmetric form $h_{A,B}$ is closed, and bounded below. Let us denote by $H_{A,B}$ the associated bounded below selfadjoint operator (see theorems 2.1 and 2.6 in chapter 6 of [32]). Note that

$$D(H_{A,B}) = \{\psi \in \mathbf{H}_{1,A,B} : -B^\dagger \psi(0) + A^\dagger \psi'(0) = 0, -\psi'' + V\psi \in L^2\}.$$

5 The Resolvent

5.1 The case of zero potential

We first consider the case of the diagonal matrices \tilde{A}, \tilde{B} given in (3.25). Let us denote by $R_{0,\tilde{A},\tilde{B}}(z)$ the resolvent of $H_{0,\tilde{A},\tilde{B}}$,

$$R_{0,\tilde{A},\tilde{B}}(z) := \left(H_{0,\tilde{A},\tilde{B}} - z\right)^{-1}, \quad z \in \rho\left(H_{0,\tilde{A},\tilde{B}}\right). \quad (5.1)$$

Let, $R_{0,\tilde{A},\tilde{B}}(z)(x, y)$ be the integral kernel of $R_{0,\tilde{A},\tilde{B}}(z)$. Then, we have that,

$$R_{0,\tilde{A},\tilde{B}}(z)(x, y) = \begin{cases} \varphi_{0,\tilde{A},\tilde{B}}(x, k) e^{iky} \left[J_{0,\tilde{A},\tilde{B}}(k)\right]^{-1}, & x \leq y, \\ e^{ikx} \varphi_{0,\tilde{A},\tilde{B}}(y, k) \left[J_{0,\tilde{A},\tilde{B}}(k)\right]^{-1}, & x \geq y, \end{cases} \quad (5.2)$$

where, $k := \sqrt{z}$, $\text{Im } k \geq 0$, and $J_{0,\tilde{A},\tilde{B}}$ is the Jost matrix given in (3.29).

We designate by $R_{0,A,B}(z)$ the resolvent of $H_{0,A,B}$. Then, by (3.24), (3.27),

$$R_{0,A,B}(z) = M R_{0,\tilde{A},\tilde{B}}(z) M^\dagger, \quad z \in \rho(H_{0,A,B}). \quad (5.3)$$

Hence, by (3.20)-(3.22) and (5.2) the integral kernel of $R_{0,A,B}(z)$ is given by,

$$R_{0,A,B}(z)(x, y) = \begin{cases} \varphi_{0,A,B}(x, k) e^{iky} [J_{0,A,B}(k)]^{-1}, & x \leq y, \\ e^{ikx} \varphi_{0,A,B}(y, k) [J_{0,A,B}(k)]^{-1}, & x \geq y. \end{cases} \quad (5.4)$$

The estimate below follows from (3.30), (3.33), (5.2) and (5.3)

$$|R_{0,A,B}(z)(x, y)| \leq CD(k) e^{-\text{Im } k|x-y|}, D(k) := \max \left[\frac{1}{|k|}, \frac{1}{|\cos \theta_1 + ik \sin \theta_1|}, \dots, \frac{1}{|\cos \theta_{n_M} + ik \sin \theta_{n_M}|} \right], k = \sqrt{z}, \quad (5.5)$$

$$\left| \frac{\partial}{\partial x} R_{0,A,B}(z)(x, y) \right| \leq CF(k) e^{-\text{Im } k|x-y|}, F(k) := \max \left[\frac{1 + |k|}{|\cos \theta_1 + ik \sin \theta_1|}, \dots, \frac{1 + |k|}{|\cos \theta_{n_M} + ik \sin \theta_{n_M}|} \right], k = \sqrt{z}.$$

It follows from (5.5) that for $z \in \mathbf{C}^\pm$, the resolvent $R_{0,A,B}(z)$ extends from $L^1 \cap L^2$ into a bounded operator in $\mathcal{B}(L^1, \mathbf{W}_{1,\infty})$. Furthermore, as

$$-\frac{d^2}{dx^2} R_{0,A,B}(z) = H_{0,A,B} R_{0,A,B}(z) = I + z R_{0,A,B}(z), \quad (5.6)$$

we have that $R_{0,A,B}(z) \in \mathcal{B}(L^1, \mathbf{W}_{2,\infty})$, with norm uniformly bounded for z in any compact set of \mathbf{C}^\pm . Furthermore, by (5.5) we also have that, $R_{0,A,B}(z) \in \mathcal{B}(L^1, L^1)$, with norm uniformly bounded for z in any compact set of \mathbf{C}^\pm . Then, for any $\psi \in L^1$,

$$\frac{d}{dz} R_{0,A,B}(z) \psi = (R_{0,A,B}(z))^2 \psi \in \mathbf{W}_{2,\infty}, \quad \forall z \in \mathbf{C}^\pm,$$

where the derivative with respect to z exists in the strong topology of $W_{2,\infty}$. Then, by Theorem 3.12 in page 152 of [32] $R_{0,A,B}(z)$ is analytic as an operator valued function from \mathbf{C}^\pm into $\mathcal{B}(L^1, \mathbf{W}_{2,\infty})$.

In the following theorem we give a limiting absorption principle for $H_{0,A,B}$

THEOREM 5.1. *For every $\lambda > 0$ the following limits,*

$$R_{0,A,B}(\lambda \pm i0) := \lim_{\varepsilon \downarrow 0} R_{0,A,B}(\lambda \pm i\varepsilon), \quad (5.7)$$

exist in the strong operator topology in $\mathcal{B}(L^1, W_{2,\infty})$. Furthermore, the functions,

$$R_{0,A,B}^\pm := \begin{cases} R_{0,A,B}(\lambda), & \text{if } \lambda \in \mathbf{C}^\pm, \\ R_{0,A,B}(\lambda \pm i0), & \text{if } \lambda \in (0, \infty), \end{cases} \quad (5.8)$$

defined for $\lambda \in \mathbf{C}^\pm \cup (0, \infty)$, with values in $\mathcal{B}(L^1, W_{2,\infty})$ are analytic for $\lambda \in \mathbf{C}^\pm$ and continuous in the strong operator topology for $\lambda \in (0, \infty)$.

Proof: the theorem follows from (5.4)-(5.6). □

Note that it follows from (5.4) that the integral kernel of $R_{0,A,B}(k^2 \pm i0)$ is given by,

$$R_{0,A,B}(k^2 \pm i0)(x, y) = \begin{cases} M \varphi_{0,\tilde{A},\tilde{B}}(x, k) \left[J_{0,\tilde{A},\tilde{B}}(\pm k) \right]^{-1} e^{\pm iky} M^\dagger, & x \leq y, \\ M e^{\pm ikx} \left[J_{0,\tilde{A},\tilde{B}}(\pm k) \right]^{-1} \varphi_{0,\tilde{A},\tilde{B}}(y, k) M^\dagger, & x \geq y. \end{cases} \quad (5.9)$$

REMARK 5.2. Equations (5.5), (5.6), (5.9) imply that, for $k^2 \in (0, \infty)$,

$$\left\| R_{0,A,B}^\pm(k^2) \right\|_{\mathcal{B}(L^1, L^\infty)} \leq \frac{C}{|k|}, \left\| R_{0,A,B}^\pm(\lambda) \right\|_{\mathcal{B}(L^1, W_{1,\infty})} \leq C \frac{1+|k|}{|k|}, \left\| R_{0,A,B}^\pm(\lambda) \right\|_{\mathcal{B}(L^1, W_{2,\infty})} \leq C \frac{1+|k|^2}{|k|}. \quad (5.10)$$

□

5.2 The case of integrable potential

Let,

$$V = \hat{U}|V|, \quad (5.11)$$

be the polar decomposition of V [32], with \hat{U} partially isometric, and $|V|$ the absolute value of V . We have that, $\hat{U} = \hat{U}^*, \hat{U}|V| = |V|\hat{U}$. Denote,

$$V_1 := \sqrt{|V|}, \quad V_2 := \hat{U}\sqrt{|V|}. \quad (5.12)$$

Since, $V_j \in L^2, j = 1, 2$ and $\mathbf{H}_1 \subset L^\infty$ we have that, $V_j \in \mathcal{B}(\mathbf{H}_1, L^2)$ and also by duality, $V_j \in \mathcal{B}(L^2, \mathbf{H}_{-1})$. Then, the quadratic form (4.11) can be written as,

$$h_{A,B}(\varphi, \psi) := h_{0,A,B}(\varphi, \psi) + (V_1 \varphi, V_2 \psi), \quad D(h_{A,B}) = \mathbf{H}_{1,A,B}. \quad (5.13)$$

Let us denote by $R_{A,B}(z) := (H_{A,B} - z)^{-1}$ the resolvent of $H_{A,B}$ for $z \in \rho(H_{A,B})$. By (5.13) with $\varphi = R_{0,A,B}(z)f, \psi = R_{A,B}(\bar{z})g$ we obtain that,

$$R_{A,B}(z) - R_{0,A,B}(z) = -R_{A,B}(z) V_2 V_1 R_{0,A,B}(z) = -R_{0,A,B}(z) V_2 V_1 R_{A,B}(z), \quad z \in \rho(H_{0,A,B}) \cap \rho(H_{A,b}). \quad (5.14)$$

As $D(H_{0,AB}) \subset \mathbf{H}_1, D(H_{A,B}) \subset \mathbf{H}_1$, it follows that, $R_{0,A,B}(z) \in \mathcal{B}(L^2, \mathbf{H}_1), R_{A,B}(z) \in \mathcal{B}(L^2, \mathbf{H}_1)$ and by duality $R_{0,A,B}(z) \in \mathcal{B}(\mathbf{H}_{-1}, L^2), R_{A,B}(z) \in \mathcal{B}(\mathbf{H}_{-1}, L^2)$.

By (5.5) $V_1 R_{0,A,B}^\pm(z) V_2$ is a Hilbert-Schmidt operator in L^2 and its Hilbert-Schmidt norm satisfies,

$$\left\| V_1 R_{0,A,B}^\pm(z) V_2 \right\|_{\text{HS}} \leq C D(k), \quad D(k) := \max \left[\frac{1}{|k|}, \frac{1}{|\cos \theta_1 + ik \sin \theta_1|}, \dots, \frac{1}{|\cos \theta_{n_M} + ik \sin \theta_{n_M}|} \right], \quad k = \sqrt{z}. \quad (5.15)$$

Hence, by (5.14)

$$(I - V_1 R_{A,B}(z) V_2) (I + V_1 R_{0,A,B}(z) V_2) \varphi = \varphi, \quad \forall \varphi \in L^2. \quad (5.16)$$

In Lemma 5.3 below we prove that $(I + V_1 R_{0,A,B}(z) V_2)$ is invertible in L^2 . Then, applying (5.16) to $\varphi = (I + V_1 R_{0,A,B}(z) V_2)^{-1} \psi$ we obtain,

$$(I - V_1 R_{A,B}(z) V_2) \psi = (I + V_1 R_{0,A,B}(z) V_2)^{-1} \psi, \quad \forall \psi \in L^2. \quad (5.17)$$

It follows that, $V_1 R_{A,B}(z) V_2 \in \mathcal{B}(L^2)$ and

$$I - V_1 R_{A,B}(z) V_2 = (I + V_1 R_{0,A,B}(z) V_2)^{-1}. \quad (5.18)$$

Iterating (5.14) and using (5.17) we prove that,

$$R_{A,B}(z) = R_{0,A,B}(z) - R_{0,A,B}(z) V_2 (I + V_1 R_{0,A,B}(z) V_2)^{-1} V_1 R_{0,A,B}(z), \quad z \in \rho(H_{0,A,B}) \cap \rho(H_{A,b}). \quad (5.19)$$

Denote,

$$Q_{\pm}(\lambda) = V_1 R_{0,A,B}^{\pm}(\lambda) V_2, \quad \lambda \in \mathbf{C}^{\pm} \cup (0, \infty). \quad (5.20)$$

LEMMA 5.3. *Suppose that V satisfies (1.6), (1.7). Then, for every $\lambda \in \mathbf{C}^{\pm} \cup (0, \infty)$ the operator $I + Q_{\pm}(\lambda)$ is invertible in L^2 .*

Proof: since $Q_{\pm}(\lambda)$ is compact we only have to prove that -1 is not an eigenvalue. On the contrary, suppose that there is a $\varphi \in L^2$ such that,

$$\varphi = -Q_{\pm}(\lambda) \varphi.$$

Denote,

$$\psi := R_{0,A,B}^{\pm}(\lambda) V_2 \varphi.$$

Then, $\psi \in L^{\infty}$, it satisfies the boundary condition (1.2) and

$$H_{A,B} \psi = \lambda \psi.$$

Moreover, ψ can be written as in (3.7) but with $\eta = 0$ because it is bounded. Then, if $\lambda \in \mathbf{C}^{\pm}$, $\psi \in L^2$ and λ would be a complex eigenvalue of $H_{A,B}$, what is impossible because $H_{A,B}$ is selfadjoint. If $\lambda \in (0, \infty)$, it follows from (5.9) that,

$$\psi = e^{\pm ikx} \xi + o(1), \quad x \rightarrow \infty, \quad \text{for some } \xi \in \mathbf{C}^n, k = \sqrt{\lambda}.$$

But then,

$$\psi - f(\pm k, x) \xi \rightarrow 0, \quad x \rightarrow \infty.$$

However, as $\psi - f(\pm k, x) \xi$ is a solution to (3.1), it is a linear combination of $f(k, x)$ and $g(k, x)$, but as $f(k, x)$ behaves as e^{ikx} and $g(k, x)$ as e^{-ikx} , $x \rightarrow \infty$ (see (3.2), (3.5)), necessarily, $\psi - f(\pm k, x) \xi = 0$. Hence,

$$\psi = f(\pm k, x) \xi,$$

and as ψ satisfies the boundary condition (1.2), it follows that,

$$0 = (-B^\dagger f(\pm k, 0) + A^\dagger f'(\pm k, 0)) \xi = -J^\dagger(\mp k) \xi.$$

This implies that $\xi = 0$ because $J^\dagger(k)$ is invertible for $k \in \mathbb{R} \setminus 0$ [6]. It follows that $\psi = 0$.

□

We give below a limiting absorption principle for $H_{A,B}$.

THEOREM 5.4. *Suppose that V satisfies (1.6), (1.7). Then, for every $\lambda > 0$ the following limits,*

$$R_{A,B}(\lambda \pm i0) := \lim_{\varepsilon \downarrow 0} R_{A,B}(\lambda \pm i\varepsilon), \quad (5.21)$$

exist in the strong operator topology in $\mathcal{B}(L^1, W_{2,\infty})$. Furthermore, the functions,

$$R_{A,B}^\pm := \begin{cases} R_{A,B}(\lambda), & \text{if } \lambda \in \mathbf{C}^\pm, \\ R_{A,B}(\lambda \pm i0), & \text{if } \lambda \in (0, \infty), \end{cases} \quad (5.22)$$

defined for $\lambda \in \mathbf{C}^\pm \cup (0, \infty)$, with values in $\mathcal{B}(L^1, W_{2,\infty})$ are analytic for $\lambda \in \mathbf{C}^\pm$ and continuous in the strong operator topology for $\lambda \in (0, \infty)$.

Proof: the theorem follows from Theorem 5.1, Lemma 5.3 and (5.19). □

Note that,

$$R_{A,B}^\pm(\lambda) = R_{0,A,B}^\pm(\lambda) - R_{0,A,B}^\pm(\lambda) V_2 (I + Q_\pm(\lambda))^{-1} V_1 R_{0,A,B}^\pm(\lambda), \quad \lambda \in \mathbf{C}^\pm \cup (0, \infty). \quad (5.23)$$

Moreover, by (5.10), (5.15) and (5.23), for every $\delta > 0$ there is a constant C_δ such that for $k^2 \in (\delta^2, \infty)$,

$$\left\| R_{A,B}^\pm(k^2) \right\|_{\mathcal{B}(L^1, L^\infty)} \leq \frac{C_\delta}{|k|}, \left\| R_{0,A,B}^\pm(k^2) \right\|_{\mathcal{B}(L^1, W_{1,\infty})} \leq C_\delta \left\| R_{0,A,B}^\pm(k^2) \right\|_{\mathcal{B}(L^1, W_{2,\infty})} \leq C_\delta |k|. \quad (5.24)$$

6 The generalized Fourier maps

6.1 The case of zero potential

It is proven in the comments at the beginning of Section VIII of [7] that $H_{0,A,B}$ has no positive or zero eigenvalues. For $\lambda \in \mathbb{R}$ we denote by $E_{0,A,B}(\lambda)$ the spectral family of $H_{0,A,B}$ and for any Borel set O we designate by $E_{0,A,B}(O)$ the spectral projector of $H_{0,A,B}$ for O .

We first consider the case of the representation where the boundary conditions (1.2) are given by the real diagonal matrices \tilde{A}, \tilde{B} (3.25). By Stone's formula, Theorem 5.1 and Remark 5.2, for all $0 < a < b$,

$$\begin{aligned} (E_{0,\tilde{A},\tilde{B}}((a,b)) \varphi, \psi) &= \lim_{\varepsilon \downarrow 0} \frac{1}{2\pi i} \int_a^b d\lambda \left([R_{0,\tilde{A},\tilde{B}}(\lambda + i\varepsilon) - R_{0,\tilde{A},\tilde{B}}(\lambda - i\varepsilon)] \varphi, \psi \right) \\ &= \frac{1}{2\pi i} \int_a^b d\lambda \left([R_{0,\tilde{A},\tilde{B}}(\lambda + i0) - R_{0,\tilde{A},\tilde{B}}(\lambda - i0)] \varphi, \psi \right) \quad \forall \varphi, \psi \in L^2 \cap L^1. \end{aligned} \quad (6.1)$$

Hence, the spectrum of $H_{0,\tilde{A},\tilde{B}}$ in $(0, \infty)$ is absolutely continuous and

$$\frac{d}{d\lambda} (E_{0,\tilde{A},\tilde{B}}(\lambda) \varphi, \psi) = \frac{1}{2\pi i} \left([R_{0,\tilde{A},\tilde{B}}(\lambda + i0) - R_{0,\tilde{A},\tilde{B}}(\lambda - i0)] \varphi, \psi \right), \quad \lambda > 0, \quad \forall \varphi, \psi \in L^2 \cap L^1. \quad (6.2)$$

Let us denote by $\psi_{0,\tilde{A},\tilde{B}}(k, x)$ the physical solution (3.13) with $A = \tilde{A}, B = \tilde{B}$ and $V = 0$.

$$\psi_{0,\tilde{A},\tilde{B}}(k, x) := -ik \varphi_{0,\tilde{A},\tilde{B}}(k, x) J_{0,\tilde{A},\tilde{B}}^{-1}(k). \quad (6.3)$$

Let $E_{0,\tilde{A},\tilde{B}}(O, x, y)$ be the integral kernel of $E_{0,\tilde{A},\tilde{B}}(O)$. Then, by (5.9) and (3.12) with $A = \tilde{A}, B = \tilde{B}, M = I$ and (6.1),

$$E_{0,\tilde{A},\tilde{B}}((k_0^2, k_1^2))(x, y) = \frac{2}{\pi} \int_{k_0}^{k_1} \psi_{0,\tilde{A},\tilde{B}}(k, x) \psi_{0,\tilde{A},\tilde{B}}^\dagger(k, y) dk, \quad (6.4)$$

where we also used that $J_{0,\tilde{A},\tilde{B}}^\dagger(k) = J_{0,\tilde{A},\tilde{B}}(-k)$, see (3.30).

Let us define,

$$\psi_{0,\tilde{A},\tilde{B}}^+(k, x) := \psi_{0,\tilde{A},\tilde{B}}(-k, x), \quad \psi_{0,\tilde{A},\tilde{B}}^-(k, x) := \psi_{0,\tilde{A},\tilde{B}}(k, x). \quad (6.5)$$

Note that,

$$\psi_{0,\tilde{A},\tilde{B}}^+(k, x) = \overline{\psi_{0,\tilde{A},\tilde{B}}(k, x)}.$$

By (3.30), (3.32), (3.33), (6.3) and (6.5),

$$\psi_{0,\tilde{A},\tilde{B}}^\pm = \text{diag}\{\psi_{0,\tilde{A},\tilde{B},1}^\pm, \psi_{0,\tilde{A},\tilde{B},2}^\pm, \dots, \psi_{0,\tilde{A},\tilde{B},n}^\pm\}, \quad (6.6)$$

$$\psi_{0,\tilde{A},\tilde{B},j}^{\pm}(k,x) = \begin{cases} \pm i \sin(kx), & \text{if } \theta_j = \pi, \\ \cos kx, & \text{if } \theta_j = \pi/2, \\ i [\pm \cos \theta_j \sin kx \mp k \sin \theta_j \cos kx] \frac{1}{\cos \theta_j \mp ik \sin \theta_j}, & \theta_j \neq \pi, \pi/2. \end{cases} \quad (6.7)$$

We denote by $F_{0,\tilde{A},\tilde{B}}^{\pm}$ the generalized Fourier maps,

$$\left(F_{0,\tilde{A},\tilde{B}}^{\pm} \psi\right)(k) := \sqrt{\frac{2}{\pi}} \int_0^{\infty} \left(\psi_{0,\tilde{A},\tilde{B}}^{\pm}(k,x)\right)^{\dagger} \psi(x) dx, \quad \psi \in L^2 \cap L^1. \quad (6.8)$$

Then, by (6.4), denoting by $\langle \cdot, \cdot \rangle$ the scalar product in \mathbf{C}^n ,

$$\left(E_{0,\tilde{A},\tilde{B}}((k_0^2, k_1^2))\psi_1, \psi_2\right) = \int_{k_0}^{k_1} \left\langle \left(F_{0,\tilde{A},\tilde{B}}^{\pm} \psi_1\right)(k), \left(F_{0,\tilde{A},\tilde{B}}^{\pm} \psi_2\right)(k) \right\rangle dk, \quad \forall \psi_1, \psi_2 \in L^2 \cap L^1, \quad (6.9)$$

where we used that $\psi_{0,\tilde{A},\tilde{B}}^{\pm}(k,x)$ are diagonal matrices and that $\varphi_{0,\tilde{A},\tilde{B}}(x,k)$ is real valued for k real. Taking the limit $k_0 \rightarrow 0, k_1 \rightarrow \infty$ with $\psi_1 = \psi_2$, we obtain that,

$$\left\|E_{0,\tilde{A},\tilde{B}}((0, \infty))\psi\right\| = \left\|F_{0,\tilde{A},\tilde{B}}^{\pm} \psi\right\|_{L^2}, \quad \forall \psi \in L^2 \cap L^1. \quad (6.10)$$

Hence, the $F_{0,\tilde{A},\tilde{B}}^{\pm}$ extend to bounded operators on L^2 .

In the next theorem we give the properties of the generalized Fourier maps, $F_{0,\tilde{A},\tilde{B}}^{\pm}$.

THEOREM 6.1. *The Hamiltonian $H_{0,\tilde{A},\tilde{B}}$ has no positive or zero eigenvalues. Its negative spectrum consists of a finite number of eigenvalues of multiplicity smaller or equal to n . The non-negative spectrum is $[0, \infty)$ and it is absolutely continuous. The generalized Fourier maps $F_{0,\tilde{A},\tilde{B}}^{\pm}$ are partially isometric with initial subspace $\mathcal{H}_{ac}(H_{0,\tilde{A},\tilde{B}})$ and final subspace L^2 . Moreover, the adjoint operators are given by,*

$$\left(\left(F_{0,\tilde{A},\tilde{B}}^{\pm}\right)^{\dagger} \psi\right)(x) = \sqrt{\frac{2}{\pi}} \int_0^{\infty} \left(\psi_{0,\tilde{A},\tilde{B}}^{\pm}(k,x)\right) \psi(k) dk, \quad \psi \in L^2 \cap L^1. \quad (6.11)$$

Furthermore,

$$F_{0,\tilde{A},\tilde{B}}^{\pm} H_{0,\tilde{A},\tilde{B}} \left(F_{0,\tilde{A},\tilde{B}}^{\pm}\right)^{\dagger} = k^2. \quad (6.12)$$

Proof: Recall that it is proven in the comments at the beginning of Section VIII of [7] that $H_{0,\tilde{A},\tilde{B}}$ has no positive or zero eigenvalues. Furthermore in Theorems 8.1 and 8.6 of [7]) it is established that it has a finite number of negative eigenvalues of multiplicity less or equal to n , that coincide with the points $-k^2$ such that $J_{0,\tilde{A},\tilde{B}}(ik)$ is not invertible for $k \in \mathbf{R}$. Let us denote by $\sigma_{0,p}$ the set of negative eigenvalues of $H_{0,\tilde{A},\tilde{B}}$. Hence, by (5.2), (5.5) the resolvent $R_{0,\tilde{A},\tilde{B}}(z)$ is a bounded operator in L^2 for $z \in (-\infty, 0) \setminus \sigma_{0,p}$, and in consequence the only spectrum in $(-\infty, 0)$ is $\sigma_{0,p}$. By (6.2) $H_{0,\tilde{A},\tilde{B}}$ has no singular continuous spectrum. It follows from (6.10) that $F_{0,\tilde{A},\tilde{B}}^{\pm}$ are partially isometric with initial subspace $E_{0,\tilde{A},\tilde{B}}((0, \infty))L^2$ into L^2 . Equation (6.11) is immediate from the definition of $F_{0,\tilde{A},\tilde{B}}^{\pm}$ in (6.8),

and (6.12) follows from the fact that $\psi_{0,\tilde{A},\tilde{B}}^\pm(k, x)$ are solution to the Schrödinger equation (3.1) But, then by (6.12) $[0, \infty)$ actually belongs to the spectrum of $H_{0,\tilde{A},\tilde{B}}$ and $\mathcal{H}_{ac}(H_{0,\tilde{A},\tilde{B}}) = E_{0,\tilde{A},\tilde{B}}((0, \infty))L^2$.

It remains to prove that the $F_{0,\tilde{A},\tilde{B}}^\pm$ are onto L^2 . Suppose, on the contrary, that there is $\phi_\pm \in L^2$ such that,

$$\left(\phi_\pm, F_{0,\tilde{A},\tilde{B}}^\pm E_{0,\tilde{A},\tilde{B}}(k_0^2, k_1^2) \psi \right) = 0, \quad \forall \psi \in L^2 \cap L^1, \forall 0 < k_0, k_1. \quad (6.13)$$

Since by (6.9),

$$\chi_{(k_0, k_1)}(k) F_{0,\tilde{A},\tilde{B}}^\pm = F_{0,\tilde{A},\tilde{B}}^\pm E_{0,\tilde{A},\tilde{B}}(k_0^2, k_1^2), \quad (6.14)$$

where $\chi_{(k_0, k_1)}$ is the characteristic function of (k_0, k_1) , it follows from (6.13) that,

$$\left(F_{0,\tilde{A},\tilde{B}}^\pm \right)^\dagger \chi_{(k_0, k_1)} \phi_\pm = \sqrt{\frac{2}{\pi}} \int_{k_0}^{k_1} \psi_{0,\tilde{A},\tilde{B}}^\pm(k, x) \phi_\pm(k) dk = 0, \quad \forall 0 < k_0 < k_1. \quad (6.15)$$

Since $\varphi_{0,\tilde{A},\tilde{B}}(k, 0) = \tilde{A}$, $\varphi'_{0,\tilde{A},\tilde{B}}(k, 0) = \tilde{B}$ it follows from (6.3), (6.5) and (6.15) that,

$$\int_{k_0}^{k_1} k (\tilde{B} + i\tilde{A}) \left(J_{0,\tilde{A},\tilde{B}}(\mp k) \right)^{-1} \phi_\pm(k) dk = 0, \quad \forall 0 < k_0 < k_1.$$

Finally since $(\tilde{B} + i\tilde{A}) \left(J_{0,\tilde{A},\tilde{B}}(\mp k) \right)^{-1}$ is invertible for $k \neq 0$ (see (3.25), (3.30)) we obtain that $\phi_\pm = 0$.

□

Let us now consider the case of A, B . We denote by $\psi_{0,A,B}(k, x)$ the physical solution (3.13) in the case $V = 0$,

$$\psi_{0,A,B}(k, x) := -ik \varphi_{0,A,B}(k, x) J_{0,A,B}^{-1}(k). \quad (6.16)$$

We define,

$$\psi_{0,A,B}^\pm(k, x) := \psi_{0,A,B}(\mp k, x). \quad (6.17)$$

By (3.21) and (3.22),

$$\psi_{0,A,B}^\pm(k, x) := M \psi_{0,\tilde{A},\tilde{B}}^\pm(k, x) M^\dagger. \quad (6.18)$$

We define the generalized Fourier maps for $A_{0,A,B}$ as,

$$\left(F_{0,A,B}^\pm \psi \right) (k) := \sqrt{\frac{2}{\pi}} \int_0^\infty \left(\psi_{0,A,B}^\pm(k, x) \right)^\dagger \psi(x) dx, \quad \psi \in L^2 \cap L^1. \quad (6.19)$$

It follows from (6.18) that,

$$F_{0,A,B}^\pm = M F_{0,\tilde{A},\tilde{B}}^\pm M^\dagger. \quad (6.20)$$

Hence, by (3.24), (3.27), (6.9) and (6.20),

$$(E_{0,A,B}((k_0^2, k_1^2))\psi_1, \psi_2) = \int_{k_0}^{k_1} \left\langle \left(F_{0,A,B}^\pm \psi_1\right)(k), \left(F_{0,A,B}^\pm \psi_2\right)(k) \right\rangle dk, \quad \forall \psi_1, \psi_2 \in L^2 \cap L^1. \quad (6.21)$$

THEOREM 6.2. *The Hamiltonian $H_{0,A,B}$ has no positive or zero eigenvalues. Its negative spectrum consists of a finite number of eigenvalues of multiplicity smaller or equal to n . The non negative spectrum is $[0, \infty)$ and it is absolutely continuous. The generalized Fourier maps $F_{0,A,B}^\pm$ partially isometric with initial subspace $\mathcal{H}_{ac}(H_{0,A,B})$ and final subspace L^2 . Moreover, the adjoint operators are given by,*

$$\left(\left(F_{0,A,B}^\pm\right)^\dagger \psi \right)(x) = \sqrt{\frac{2}{\pi}} \int_0^\infty \left(\psi_{0,A,B}^\pm(k, x) \right) \psi(k) dk, \quad \psi \in L^2 \cap L^1. \quad (6.22)$$

Furthermore,

$$F_{0,A,B}^\pm H_{0,A,B} \left(F_{0,A,B}^\pm\right)^\dagger = k^2. \quad (6.23)$$

Proof: The theorem follows from (3.24), (3.27), Theorem 6.1 and (6.20). □

6.2 The case of integrable potential.

It is proven in the comments at the beginning of Section VIII of [7] that $H_{A,B}$ has no positive or zero eigenvalues. We denote,

$$L_{A,B}^\pm(\lambda) := I - V R_{A,B}^\pm(\lambda), \quad \lambda \in \mathbf{C}^\pm \cup (0, \infty). \quad (6.24)$$

Then, by Theorem 5.1 and (5.14),

$$R_{A,B}^\pm(\lambda) = R_{0,A,B}^\pm(\lambda) L_{A,B}^\pm(\lambda), \quad \lambda \in \mathbf{C}^\pm \cup (0, \infty). \quad (6.25)$$

Since,

$$R_{A,B}(z) - R_{A,B}(\bar{z}) = (z - \bar{z}) R_{A,B}(z) R_{A,B}(\bar{z}), \quad z \in \mathbf{C}^\pm,$$

Then,

$$\frac{1}{2\pi i} [R_{A,B}(z) - R_{A,B}(\bar{z})] = \left(L_{A,B}^+\right)^*(z) \frac{1}{2\pi i} [R_{0,A,B}(z) - R_{0,A,B}(\bar{z})] L_{A,B}^+(z), \quad z \in \mathbf{C}^+, \quad (6.26)$$

and also,

$$R_{A,B}(z) - R_{A,B}(\bar{z}) = (z - \bar{z}) R_{A,B}(\bar{z}) R_{A,B}(z), \quad z \in \mathbf{C}^\pm,$$

we have that,

$$\frac{1}{2\pi i} [R_{A,B}(z) - R_{A,B}(\bar{z})] = \left(L_{A,B}^-\right)^*(\bar{z}) \frac{1}{2\pi i} [R_{0,A,B}(z) - R_{0,A,B}(\bar{z})] L_{A,B}^-(\bar{z}), \quad z \in \mathbf{C}^+. \quad (6.27)$$

We define the generalized Fourier maps for $H_{A,B}$ as follows,

$$\left(F_{A,B}^\pm \psi\right)(k) := \sqrt{\frac{2}{\pi}} \int_0^\infty \left(\psi_{0,A,B}^\pm(k, x)\right)^\dagger L^\pm(k^2) \psi(x) dx, \quad \psi \in L^2 \cap L^1. \quad (6.28)$$

For $\lambda \in \mathbb{R}$ we denote by $E_{A,B}(\lambda)$ the spectral family of $H_{A,B}$ and for any Borel set O let us designate by $E_{A,B}(O)$ the spectral projector of $H_{A,B}$ for O . Then, by Theorems 5.4, 6.1, (6.21), (6.26), (6.27) and Stone's formula we have that,

$$(E_{A,B}((k_0^2, k_1^2))\psi_1, \psi_2) = \int_{k_0}^{k_1} \left\langle \left(F_{A,B}^\pm \psi_1\right)(k), \left(F_{A,B}^\pm \psi_2\right)(k) \right\rangle dk, \quad \forall \psi_1, \psi_2 \in L^2 \cap L^1, \forall 0 < k_0 < k_1, \quad (6.29)$$

where we used that $H_{A,B}$ has no positive or zero eigenvalues.

Taking the limit $k_0 \rightarrow 0, k_1 \rightarrow \infty$ in (6.29) with $\psi_1 = \psi_2 = \psi$ we get that,

$$\left\| F_{A,B}^\pm \psi \right\|_{L^2} = \|E_{A,B}([0, \infty))\psi\|_{L^2}. \quad (6.30)$$

Then, the $F_{A,B}^\pm$ extend to bounded operators in L^2 .

THEOREM 6.3. *Suppose that V satisfies (1.6), (1.7). Then, $H_{A,B}$ has no zero or positive eigenvalues, and the negative spectrum of $H_{A,B}$ consists of isolated eigenvalues of multiplicity smaller or equal than n , that can accumulate only at zero. Furthermore, $H_{A,B}$ has no singular continuous spectrum and its absolutely continuous spectrum is given by $[0, \infty)$. The generalized Fourier maps $F_{A,B}^\pm$ are partially isometric with initial subspace $\mathcal{H}_{ac}(H_{A,B})$ and final subspace L^2 . Moreover, the adjoint operators are given by,*

$$\left(\left(F_{A,B}^\pm\right)^\dagger \psi\right)(x) = \sqrt{\frac{2}{\pi}} \int_0^\infty \left(L^\pm(k^2)\right)^\dagger \psi_{0,A,B}^\pm(k, x) \psi(k) dk, \quad \psi \in L^2 \cap L^1. \quad (6.31)$$

Furthermore,

$$F_{A,B}^\pm H_{A,B} \left(F_{A,B}^\pm\right)^\dagger = k^2. \quad (6.32)$$

Proof: Recall that it is proven in the comments at the beginning of Section VIII of [7] that $H_{A,B}$ has no positive or zero eigenvalues. In Lemma 9.1 in Section 9 we prove that for all $z \in \rho(H_{0,A,B}) \cap \rho(H_{A,B})$ the difference of the resolvents of $H_{0,A,B}$ and $H_{A,B}$ is trace class. Then, the essential spectrum of $H_{A,B}$ is $[0, \infty)$ and the negative spectrum consists of isolated eigenvalues of finite multiplicity that can accumulate only at zero. It follows from item (b) of Theorem 8.1 in [7] that the multiplicities of the eigenvalues is smaller or equal to n . Note that in Section 8 of [7] the condition that the potential has a finite first moment is only used in order that the number of eigenvalues is finite. By (6.29) $H_{A,B}$ has no singular continuous spectrum. The fact that the $F_{A,B}^\pm$ are partially isometric with initial subspace $\mathcal{H}_{ac}(H_{A,B})$ into L^2 and (6.32) follow from (6.29) and (6.30). Equation (6.31) follows from the definition of $F_{A,B}^\pm$ in (6.28). Equation (6.32) is implied by (6.29).

It remains to prove that the $F_{A,B}^\pm$ are onto L^2 .

By (5.14) and Theorems 5.1, and 5.4,

$$L^\pm(\lambda) \left(I + V R_{0,A,B}^\pm(\lambda) \right) = I, \quad \forall \lambda \in \mathbf{C}^\pm \cup (0, \infty), \quad (6.33)$$

as bounded operators on L^1 . Let us prove that $V R_{0,A,B}^\pm(\lambda)$ is compact in L^1 . Let ψ_n be a bounded sequence in L^1 . Since $R_{0,A,B}^\pm(\lambda) \in \mathcal{B}(L^1, W_{2,\infty})$ the sequence $R_{0,A,B}^\pm(\lambda)\psi_n$ is uniformly equicontinuous in $[0, R]$ for any $R > 0$. Then, by the Arzelà-Ascoli theorem there is a subsequence ψ_{n_l} of ψ_n such that $R_{0,A,B}^\pm(\lambda)\psi_{n_l}$ converges uniformly in $C([0, R])$ and then, $\chi_{[0,R]}(x)V(x)R_{0,A,B}^\pm(\lambda)\psi_{n_l}$ converges in L^1 . Hence the operator $\chi_{[0,R]}(x)V(x)R_{0,A,B}^\pm(\lambda)$ is compact, but since

$$\left\| V(x)R_{0,A,B}^\pm(\lambda) - \chi_{[0,R]}(x)V(x)R_{0,A,B}^\pm(\lambda) \right\|_{\mathcal{B}(L^1)} \leq C \left\| \chi_{(R,\infty)}(x)V(x) \right\|_{L^1} \rightarrow 0, \text{ as } R \rightarrow \infty,$$

it follows that $V(x)R_{0,A,B}^\pm(\lambda)$ is compact. Suppose that for some $\lambda \in \mathbf{C}^\pm \cup (0, \infty)$, $\left(I + V R_{0,A,B}^\pm(\lambda) \right)$ is not injective in L^1 . Then, by duality, also $\left(I + R_{0,A,B}^\mp(\bar{\lambda})V \right)$ is not injective in L^∞ . In consequence, there is a $\psi \in L^\infty$ such that,

$$\psi = -R_{0,A,B}^\mp(\bar{\lambda})V\psi. \quad (6.34)$$

But then, $\phi := V_1\psi \in L^2$, satisfies (recall that $V_1V_2 = V_2V_1 = V$),

$$\phi = -Q_\mp(\bar{\lambda})\phi.$$

By Lemma 5.3, $\phi = 0$ and then, by (6.34) $\psi = 0$. Hence, $\left(I + V R_{0,A,B}^\pm(\lambda) \right)$ have a bounded inverse in L^1 and by (6.33) the $L^\pm(\lambda)$ are bounded invertible in L^1 and

$$(L^\pm(\lambda))^{-1} = \left(I + V R_{0,A,B}^\pm(\lambda) \right)^{-1}, \quad \forall \lambda \in \mathbf{C}^\pm \cup (0, \infty). \quad (6.35)$$

It follows that $L^\pm(\lambda)$ are injective and onto L^2 .

Suppose that ϕ is orthogonal to the range of $F_{A,B}^\pm$. Let $\{\psi_n\}_{n=1}^\infty$ be a set of functions in $L^2 \cap L^1$ that is countable dense in L^1 . Then for all $0 < k_0 < k_1$

$$\left(\phi, F_{A,B}^\pm E_{A,B}(k_0^2, k_1^2)\psi_n \right) = \sqrt{\frac{2}{\pi}} \int_{k_0}^{k_1} dk \left(\psi_{0,A,B}^\pm(k, \cdot) \phi(k), L^\pm(k^2)\psi_n \right) = 0.$$

It follows that there is a set of measure zero, O , independent of n such that,

$$\left(\psi_{0,A,B}^\pm(k, \cdot) \phi(k), L^\pm(k^2)\psi_n \right) = 0, \forall k \in (0, \infty) \setminus O.$$

But since $L^\pm(k^2)$ is onto, also $\{L^\pm(k^2)\psi_n\}_{n=1}^\infty$ is countably dense in L^1 . Hence,

$$\psi_{0,A,B}^\pm(k, x) \phi(k) = 0, \forall k \in (0, \infty) \setminus O.$$

Finally this implies that $\| \left(F_{0,A,B}^\pm \right)^* \phi \| = \|\phi\| = 0$.

□

Let us define,

$$\psi_{A,B}^\pm(k, x) := \psi_{0,A,B}^\pm(k, x) - R_{A,B}(k^2 \mp i0) V \psi_{0,A,B}^\pm(k, x). \quad (6.36)$$

LEMMA 6.4. *Suppose that V satisfies (1.6), (1.7). Then, with $\psi_{A,B}$ defined in (3.13),*

$$\psi_{A,B}^\pm(k, x) = \psi_{A,B}(\mp k, x). \quad (6.37)$$

Proof: By (6.28), (6.31),

$$\left(F_{A,B}^\pm \psi \right) (k) = \sqrt{\frac{2}{\pi}} \int_0^\infty \left(\psi_{A,B}^\pm(k, x) \right)^\dagger \psi(x) dx, \quad \psi \in L^2 \cap L^1, \quad (6.38)$$

$$\left(\left(F_{A,B}^\pm \right)^\dagger \psi \right) (x) = \sqrt{\frac{2}{\pi}} \int_0^\infty \psi_{A,B}^\pm(k, x) \psi(k) dk, \quad \psi \in L^2 \cap L^1. \quad (6.39)$$

Furthermore, by (5.9), (6.6), (6.7), (6.18)(6.25), (6.36)

$$\psi_{A,B}^\pm(k, x) = \frac{1}{2} e^{\pm i k x} + e^{\mp i k x} D_\pm(k) + o(1), \quad \text{as } x \rightarrow \infty, \quad (6.40)$$

for a matrix $D(k)$. Let us define,

$$\phi^\pm(k, x) := \frac{1}{2} f(\pm k, x) + f(\mp k, x) D_\pm(k).$$

Then, $\psi_{A,B}^\pm(k, x) - \phi^\pm(k, x)$ is a solution to (3.1) and by (3.2), (6.40), it goes to zero as $x \rightarrow \infty$. Moreover, it is a linear combination of $f(k, x)$ and $g(k, x)$ (recall that the combined $2n$ columns of $f(k, x)$ and of $g(k, x)$ form a fundamental set of solutions to (3.1)). As $f(k, x)$ behaves as $e^{i k x}$ and $g(k, x)$ behaves as $e^{-i k x}$, as $x \rightarrow \infty$, necessarily, $\psi_{A,B}^\pm(k, x) - \phi^\pm(k, x) = 0$, and then,

$$\psi_{A,B}^\pm(k, x) = \frac{1}{2} f(\pm k, x) + f(\mp k, x) D_\pm(k). \quad (6.41)$$

Hence, by (3.16) $\chi^\pm(k, x) := \psi_{A,B}^\pm(k, x) - \psi_{A,B}(\mp k, x) = f(\mp k, x)(D_\pm(k) - \frac{1}{2} S(\mp k))$. As $\chi^\pm(k, x)$ satisfies the boundary condition (1.2), by (3.11),

$$-B^\dagger \chi^\pm(k, 0) + A^\dagger \chi^{\pm'}(k, 0) = -J_{A,B}^\dagger(\pm k)(D_\pm(k) - \frac{1}{2} S(\mp k)) = 0.$$

But as $J_{A,B}^\dagger(k)$ is invertible for $k \in \mathbb{R} \setminus 0$, $D_\pm(k) = \frac{1}{2} S(\mp k)$, and then, by (3.16), (6.41),

$$\psi_{A,B}^\pm(k, x) = \psi_{A,B}(\mp k, x). \quad (6.42)$$

7 The Wave operators

We take as unperturbed operator $H_0 := H_{-I,0}$, with the Neumann boundary condition, $\varphi'(0) = 0$. If we interpret the matrix Schrödinger operator as a star graph with one vertex the Neumann boundary condition corresponds physically to the case where there is no transfer of current between the different wires of the graph, what is a natural unperturbed boundary condition. We denote by F_0 the generalized Fourier map of H_0 , i.e., $F_0 = F_{0,-I,0}^\pm$. Note that $F_{0,-I,0}^+ = F_{0,-I,0}^-$ and that F_0 is just the cosine transform,

$$(F_0\psi)(k) := \sqrt{\frac{2}{\pi}} \int_0^\infty \cos(kx) \psi(x) dx, \quad \psi \in L^2. \quad (7.1)$$

Furthermore, H_0 has no eigenvalues.

7.1 The case of zero potential

THEOREM 7.1. *The wave operators $W_\pm(H_{0,A,B}, H_0)$ exist and are complete, they are isometric with initial subspace L^2 and final subspace $\mathcal{H}_{ac}(H_{0,A,B})$. Furthermore,*

$$W_\pm(H_{0,A,B}, H_0) = \left(F_{0,A,B}^\pm\right)^\dagger F_0. \quad (7.2)$$

Proof: Once formula (7.2) is proven, the fact that $W_\pm(H_{0,A,B}, H_0)$ are isometric with initial subspace L^2 and final subspace $\mathcal{H}_{ac}(H_{0,A,B})$ follows from Theorem 6.2. By (6.23), (6.32) it is enough to prove that,

$$\left\| \left[\left(F_{0,A,B}^\pm\right)^\dagger - F_0^\dagger \right] e^{-itk^2} \phi(k) \right\| \rightarrow 0, \text{ as } t \rightarrow \pm\infty, \quad \forall \phi \in C_0^\infty((0, \infty)). \quad (7.3)$$

But, by (6.6), (6.7), (6.11), (6.18), (6.19) and (7.1) this is equivalent to,

$$\left\| \int_0^\infty e^{\mp ikx} e^{-itk^2} \phi(k) dk \right\| \rightarrow 0, \text{ as } t \rightarrow \pm\infty, \quad \forall \phi \in C_0^\infty((0, \infty)). \quad (7.4)$$

Equation (7.4) holds by Lemma 2.6.4 of [26].

7.2 The relative wave operators

We consider now the relative wave operators $W_\pm(H_{A,B}, H_{0,A,B})$ that will allow us to obtain the wave operators with integrable potential by the chain rule, $W_\pm(H_{A,B}, H_0) = W_\pm(H_{A,B}, H_{0,A,B}) W_\pm(H_{0,A,B}, H_0)$.

THEOREM 7.2. *Suppose that V satisfies (1.6), (1.7). Then, the wave operators $W_\pm(H_{A,B}, H_{0,A,B})$ exist and are complete, they are partially isometric with initial subspace $\mathcal{H}_{ac}(H_{0,A,B})$ and final subspace $\mathcal{H}_{ac}(H_{A,B})$. Furthermore,*

$$W_\pm(H_{A,B}, H_{0,A,B}) = \left(F_{A,B}^\pm\right)^\dagger F_{0,A,B}^\pm. \quad (7.5)$$

Proof: Once (7.5) is proven, the rest of the theorem follows from Theorems 6.2 and 6.3. We prove (7.5) for $W_+(H_{A,B}, H_{0,A,B})$. The case $W_-(H_{A,B}, H_{0,A,B})$ similar. Since $\|e^{itH_{A,B}} e^{-itH_{0,A,B}} \phi\| = \left\| \left(F_{A,B}^\pm \right)^\dagger F_{0,A,B}^\pm \phi \right\| = \|\phi\|$, for all $\phi \in \mathcal{H}_{\text{ac}}(H_{0,A,B})$ it is enough to prove that

$$\lim_{t \rightarrow \infty} (e^{-itH_{A,B}} E_{A,B}(O_0) \psi_0, e^{-itH_{0,A,B}} E_{0,A,B}(O_1) \psi_1) = \left(F_{A,B}^+ E_{A,B}(O_0) \psi_0, F_{0,A,B}^+ E_{0,A,B}(O_1) \psi_1 \right), \quad (7.6)$$

for all $O_0 = (k_0^2, k_1^2), O_1 = (k_2^2, k_3^2), 0 < k_0 < k_1, 0 < k_2 < k_3$ and all $\psi_0, \psi_1 \in L^2 \cap L^1$.

By (5.20), (6.25), for $\lambda > 0$,

$$R_{A,B}(\lambda + i\varepsilon) - R_{A,B}(\lambda - i\varepsilon) = [R_{0,A,B}(\lambda + i\varepsilon) - R_{0,A,B}(\lambda - i\varepsilon)] L^+(\lambda + i\varepsilon) + R_{0,A,B}(\lambda - i\varepsilon) V_1 J(\lambda + i\varepsilon), \quad (7.7)$$

where, $L^+(\lambda + i\varepsilon)$ is defined in (6.24) and

$$J(\lambda + i\varepsilon) := -V_2 [R_{A,B}(\lambda + i\varepsilon) - R_{A,B}(\lambda - i\varepsilon)]. \quad (7.8)$$

Then, by Stone's formula,

$$\frac{d}{d\lambda} (E_{A,B}(\lambda) \psi_0, e^{-itH_{0,A,B}} E_{0,A,B}(O_1) \psi_1) = \lim_{\varepsilon \rightarrow 0} T_1(\varepsilon) + \lim_{\varepsilon \rightarrow 0} T_2(\varepsilon), \quad (7.9)$$

where,

$$T_1(\varepsilon) := \left(L^+(\lambda + i\varepsilon) E_{A,B}(\lambda) \psi_0, \frac{1}{2\pi i} [R_{0,A,B}(\rho + i0) - R_{0,A,B}(\rho - i0)] e^{-itH_{0,A,B}} E_{0,A,B}(O_1) \psi_1 \right), \quad (7.10)$$

$$T_2(\varepsilon) := \frac{1}{2\pi i} \left(J(\lambda + i\varepsilon) \psi_0, \int_{O_1} \frac{e^{-it\rho}}{\rho - (\lambda + i\varepsilon)} \frac{1}{2\pi i} V_1 [R_{0,A,B}(\rho + i0) - R_{0,A,B}(\rho - i0)] \psi_1 \right) d\rho, \quad (7.11)$$

where we used Theorem 5.1. By (6.19), (6.21), and (6.29) we have that,

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} T_1(\varepsilon) &= e^{it\lambda} \chi_{O_1}(\lambda) \left(L^+(\lambda) \psi_0, \frac{1}{2\pi i} [R_{0,A,B}(\lambda + i0) - R_{0,A,B}(\lambda - i0)] \psi_1 \right) \\ &= \frac{1}{2\sqrt{\lambda}} e^{it\lambda} \chi_{O_1}(\lambda) \left\langle \left(F_{A,B}^+ \psi_0 \right) (\sqrt{\lambda}), \left(F_{0,A,B}^+ \psi_1 \right) (\sqrt{\lambda}) \right\rangle. \end{aligned} \quad (7.12)$$

Let us denote,

$$I_t(\lambda, \varepsilon) := \int_{O_1} \frac{e^{-it\rho}}{\rho - (\lambda + i\varepsilon)} G(\rho), \quad (7.13)$$

where,

$$G(\rho) := \frac{1}{2\pi i} V_1 [R_{0,A,B}(\rho + i0) - R_{0,A,B}(\rho - i0)] \psi_1 \in L^2.$$

Then, denoting by F the Fourier transform in $L^2(\mathbb{R}, L^2)$, it follows that,

$$I_t(\lambda) := \lim_{\varepsilon \rightarrow 0} I_t(\lambda, \varepsilon) = F^{-1} (2\pi i \chi_{(0,\infty)}(k) [F \chi_{O_1}(\rho) e^{-it\rho} G(\rho)](k))(\lambda), \quad (7.14)$$

where the limit exists in $L^2(\mathbb{R}, L^2)$. Hence, by (7.9), (7.12), (7.13) and (7.14)

$$(e^{-itH_{A,B}} E_{A,B}(O_0) \psi_0, e^{-itH_{0,A,B}} E_{0,A,B}(O_1) \psi_1) = \int_{O_0} e^{-it\lambda} \frac{d}{d\lambda} (E_{A,B}(\lambda) \psi_0, e^{-itH_{0,A,B}} E_{0,A,B}(O_1) \psi_1) d\lambda =$$

$$\begin{aligned} \int \chi_{O_0 \cap O_1}(k^2) \left\langle \left(F_{A,B}^+ \psi_0 \right) (k), \left(F_{0,A,B}^+ \psi_1 \right) (k) \right\rangle dk + \frac{1}{2\pi i} \int_{O_0} (J(\lambda + i0) \psi_0, I_t(\lambda)) = \\ \left(F_{A,B}^+ E_{A,B}(O_0) \psi_0, F_{0,A,B}^+ E_{A,B}(O_1) \psi_1 \right) + \frac{1}{2\pi i} \int_{O_0} (J(\lambda + i0) \psi_0, I_t(\lambda)). \end{aligned} \quad (7.15)$$

Furthermore,

$$\|I_t(\rho)\|_{L^2(\mathbb{R}, L^2)}^2 = 4\pi^2 \int_t^\infty \|(F[\chi_{O_1}(\rho)G(\rho)])(k)\|_{L^2}^2 dk \rightarrow 0 \text{ as } t \rightarrow \infty,$$

and then,

$$\lim_{t \rightarrow \infty} \int_{O_0} (J(\lambda + i0) \psi_0, I_t(\lambda)) = 0. \quad (7.16)$$

By (7.15) and (7.16) equation (7.6) holds.

7.3 The wave operators

THEOREM 7.3. *Suppose that V satisfies (1.6), (1.7). Then, the wave operators $W_\pm(H_{A,B}, H_0)$ exist and are complete, they are isometric with initial subspace L^2 and final subspace $\mathcal{H}_{ac}(H_{A,B})$. Furthermore,*

$$W_\pm(H_{A,B}, H_0) = \left(F_{A,B}^\pm \right)^\dagger F_0. \quad (7.17)$$

Proof: By the chain rule,

$$W_\pm(H_{A,B}, H_0) = W_\pm(H_{A,B}, H_{0,A,B}) W_\pm(H_{0,A,B}, H_0).$$

Then, the theorem follows from Theorems 7.1 and 7.2.

□

8 The scattering operator and the scattering matrix

The scattering operator is defined as,

$$\mathcal{S}_{A,B} := (W_+(H_{A,B}, H_0))^\dagger W_-(H_{A,B}, H_0). \quad (8.1)$$

By theorem 7.3 \mathcal{S} is unitary in L^2 and,

$$\mathcal{S}_{A,B} = F_0^\dagger F_{A,B}^+ \left(F_{A,B}^- \right)^\dagger F_0. \quad (8.2)$$

We denote,

$$\hat{\mathcal{S}}_{A,B} := F_0 \mathcal{S}_{A,B} F_0^\dagger = F_{A,B}^+ \left(F_{A,B}^- \right)^\dagger. \quad (8.3)$$

Since $\hat{\mathcal{S}}_{A,B}$ commutes with H_0 it decomposes as a direct integral in the spectral representation of H_0 . Then, for $k \in (0, \infty)$, there is a unitary $n \times n$ matrix $\hat{\mathcal{S}}_{A,B}(k)$, such that,

$$\left(\hat{\mathcal{S}}_{A,B} \psi \right) (k) = \hat{\mathcal{S}}_{A,B}(k) \psi(k), \quad \forall \psi \in L^2. \quad (8.4)$$

Recall that the scattering matrix $S_{A,B}(k)$ was defined in (3.14).

THEOREM 8.1. *Suppose that V satisfies (1.6), (1.7). Then,*

$$\hat{\mathcal{S}}_{A,B}(k) = S_{A,B}(k), k \in (0, \infty). \quad (8.5)$$

Proof: By (6.38), (6.39), (6.42), (8.3) and (8.4)

$$\hat{\mathcal{S}}_{A,B}(k) \left(\psi_{A,B}^-(k, x) \right)^\dagger = \left(\psi_{A,B}^+(k, x) \right)^\dagger,$$

and then,

$$\psi_{A,B}^-(k, x) \hat{\mathcal{S}}_{A,B}^\dagger(k) = \psi_{A,B}^+(k, x). \quad (8.6)$$

Hence, by (3.15), (6.42),

$$f(-k, x) \left[\hat{\mathcal{S}}_{A,B}^\dagger(k) - S_{A,B}^\dagger(k) \right] = -f(k, x) \left[S_{A,B}(k) \hat{\mathcal{S}}_{A,B}^\dagger(k) - I \right].$$

but, as $f(\pm k, x) \approx e^{\pm ikx}$, $x \rightarrow \infty$, we have that, $\hat{\mathcal{S}}_{A,B}(k) = S_{A,B}(k)$.

□

By (3.7)

$$\varphi_{A,B}(k, x) = f(k, x) \alpha + g(k, x) \beta.$$

Then, by (3.3), (3.4) (3.6),

$$\alpha = \frac{1}{2ik} \left[g(-k^*, x)^\dagger; \varphi_{A,B}(k, x) \right], \quad \beta = -\frac{1}{2ik} J_{A,B}(k).$$

It follows that, for $\text{Im } k > 0$,

$$\lim_{x \rightarrow \infty} e^{ikx} \left[\varphi'_{A,B}(k, x) - ik \varphi_{A,B}(k, x) \right] = J_{A,B}(k). \quad (8.7)$$

Then, by (3.1), (3.8), (3.28) and (8.7), for $\text{Im } k > 0$,

$$\begin{aligned} \int_0^\infty e^{ikx} V(x) \varphi_{A,B}(k, x) dx &= \lim_{x \rightarrow \infty} \int_0^x e^{ikx} V(x) \varphi_{A,B}(k, x) dx \\ \int_0^x e^{ikx} \left(\varphi''_{A,B}(k, x) + k^2 \varphi_{A,B}(k, x) \right) dx &= J_{A,B}(k) - J_{0,A,B}(k), \end{aligned} \quad (8.8)$$

where in (8.8) we integrated twice by parts. Then, by continuity in k

$$J_{A,B}(k) = J_{0,A,B}(k) + \int_0^\infty e^{ikx} V(x) \varphi_{A,B}(k, x) dx, k \in \overline{\mathbf{C}^+}. \quad (8.9)$$

PROPOSITION 8.2. *Suppose that V satisfies (1.6), (1.7). Then,*

$$S_{A,B}(k) = S_{0,A,B}(k) - \frac{2i}{k} \int_0^\infty \psi_{0,A,B} V(x) \psi_{A,B}(k, x) dx, k \in \mathbb{R} \setminus 0. \quad (8.10)$$

Proof By (3.13), (3.14), (3.16) with $V = 0$, (3.28) and (8.9)

$$\int_0^\infty \psi_{0,A,B} V(x) \psi_{A,B}(k, x) dx = -\frac{ik}{2} (-S_{A,B}(k) + S_{0,A,B}(k)). \quad (8.11)$$

Equation (8.10) follows from (8.11).

9 The spectral shift function

Lets us denote by $R_0(z)$ the resolvent of H_0 , i.e. $R_0(z) := (H_0 - z)^{-1}$, $z \in \rho(H_0)$.

LEMMA 9.1. *Suppose that V satisfies (1.6), (1.7). Then, for every $z \in \rho(H_{A,B}) \cap \rho(H_{0,A,B})$ the difference of resolvents, $R_{A,B}(z) - R_{0,A,B}(z)$ is trace class and for every $z \in \rho(H_{0,A,B}) \cap \rho(H_0)$, $R_{0,A,B}(z) - R_0(z)$ is trace class.*

Proof: By (5.5) $V_2 R_{0,A,B}(z)$ is Hilbert-Schmidt. Since $D(H_{A,B})$ is contained in \mathbf{H}_1 and the imbedding of \mathbf{H}_1 into L^∞ is bounded (see (4.7)),

$$|(R_{A,B}(z)\varphi)(x)| \leq C\|\varphi\|_{L^2}, \quad \forall x \in \mathbb{R}^+.$$

Then, by the Riez representation theorem, for all $x \in \mathbb{R}^+$ there is a $\psi_x \in L^2$ such that,

$$(R_{A,B}(z)\varphi)(x) = (\varphi, \psi_x),$$

and

$$\|\psi_x\|_{L^2} \leq C, \quad \forall x \in \mathbb{R}^+.$$

Hence, $V_1 R_{A,B}(z)$ is an integral operator with the Hilbert-Schmidt kernel,

$$V_1(x) \psi_x(y), \quad x, y \in \mathbb{R}^+.$$

Hence, $V_1 R_{A,B}(z)$ is Hilbert-Schmidt. Furthermore as $V_1 R_{A,B}(z)$ and $V_2 R_{0,A,B}(z)$ are Hilbert-Schmidt, by (5.14) $R_{A,B}(z) - R_{0,A,B}(z)$ is trace class.

Furthermore using the identity,

$$\left(-\frac{d^2}{dx^2}\varphi, \psi\right) - \left(\varphi, -\frac{d^2}{dx^2}\psi\right) = \varphi'(0)\overline{\psi}(0) - \varphi(0)\overline{\psi'}(0), \quad \varphi, \psi \in \mathbf{H}_2,$$

with $\varphi = R_0(z)f$, $\psi = R_{0,A,B}(\overline{z})g$, $f, g \in L^2$ we prove that

$$R_{0,A,B}(z) - R_0(z) = (TR_{0,A,B}(\overline{z}))^\dagger \left(T\frac{d}{dx}R_0(z)\right) - \left(T\frac{d}{dx}R_{0,A,B}(\overline{z})\right)^\dagger (TR_0(z)),$$

where T is the bounded trace operator from \mathbf{H}_1 into \mathbf{C}^n ,

$$T\varphi = \varphi(0).$$

Furthermore, since H_0 has Neumann boundary condition, $T\frac{d}{dx}R_0(z) = 0$. Hence,

$$R_{0,A,B}(z) - R_0(z) = -\left(T\frac{d}{dx}R_{0,A,B}(\overline{z})\right)^\dagger (TR_0(z)).$$

Let us denote by $K(z) := T R_0(z)$, $N(\bar{z}) := T \frac{d}{dx} R_{0,A,B}(\bar{z})$. Then by (5.5), $K(z)$ and $N(\bar{z})$ are Hilbert-Schmidt and

$$\|K(z)\|_2 \leq CD(\sqrt{z}) \frac{1}{\sqrt{\operatorname{Im} \sqrt{z}}}, \quad \|N(\bar{z})\|_2 \leq CF(\sqrt{\bar{z}}) \frac{1}{\sqrt{\operatorname{Im} \sqrt{\bar{z}}}}.$$

Hence, $R_{0,A,B}(z) - R_0(z)$ is trace class and

$$\|R_{0,A,B}(z) - R_0(z)\|_1 \leq CD(\sqrt{z}) F(\sqrt{\bar{z}}) \frac{1}{\operatorname{Im} \sqrt{z}}. \quad (9.1)$$

□

For later use, we note that for all $\alpha > 1/4$

$$\|R_{A,B}(-E) - R_{0,A,B}(-E)\|_1 \leq C E^{-2+2\alpha}, \text{ as } E \rightarrow \infty. \quad (9.2)$$

This estimate is proven as in the proof of Lemma 5.6 in page 194 of [27], observing that $|V|^{1/2} (H_0 + I)^{-\alpha}$ is Hilbert-Schmidt for $\alpha > 1/4$. Indeed, with F_0 as in (7.1), $|V|^{1/2} (H_0 + I)^{-\alpha} = |V|^{1/2} F_0^\dagger (k^2 + 1)^{-\alpha} F_0$, and the operator $|V|^{1/2} F_0^\dagger (k^2 + 1)^{-\alpha}$ is an integral operator with the Hilbert-Schmidt kernel $\sqrt{\frac{2}{\pi}} |V(x)|^{1/2} \cos(kx) (k^2 + 1)^{-\alpha}$.

For any pair of self-adjoint operators F, G we denote their spectral shift function by $\xi(E; F, G)$.

As the difference of the resolvents, respectively, of $H_{A,B}$ and H_0 , $H_{0,A,B}$ and H_0 , $H_{A,B}$ and $H_{0,A,B}$, are trace class we can use the abstract theory of section 9 of chapter 0 of [27] to define their spectral shift functions as in equation (9.26), page 50 of [27]. Take $E_0 > 0$ such that, $H_{A,B} + E_0 > 0$, $H_{0,A,B} + E_0 > 0$. Since $H_0 \geq 0$, we also have that $H_0 + E_0 > 0$. Then,

$$\xi(E; H_{A,B}, H_0) = -\xi\left((E + E_0)^{-1}; (H_{A,B} + E_0)^{-1}, (H_0 + E_0)^{-1}\right), \quad E \geq E_0, \quad (9.3)$$

$$\xi(E; H_{A,B}, H_0) = 0, \quad E < E_0, \quad (9.4)$$

$$\xi(E; H_{0,A,B}, H_0) = -\xi\left((E + E_0)^{-1}; (H_{0,A,B} + E_0)^{-1}, (H_0 + E_0)^{-1}\right), \quad E \geq E_0, \quad (9.5)$$

$$\xi(E; H_{0,A,B}, H_0) = 0, \quad E < E_0, \quad (9.6)$$

$$\xi(E; H_{A,B}, H_{0,A,B}) = -\xi\left((E + E_0)^{-1}; (H_{A,B} + E_0)^{-1}, (H_{0,A,B} + E_0)^{-1}\right), \quad E \geq E_0, \quad (9.7)$$

$$\xi(E; H_{A,B}, H_{0,A,B}) = 0, \quad E < E_0. \quad (9.8)$$

By the addition formula for the spectral shift function (see Proposition 5 in page 275 of [26]),

$$\xi(E; H_{A,B}, H_0) = \xi(E; H_{A,B}, H_{0,A,B}) + \xi(E; H_{0,A,B}, H_0). \quad (9.9)$$

Furthermore, we have that,

$$\int_{-\infty}^{\infty} |\xi(E; H_{A,B}, H_{0,A,B})| (1 + |E|)^{-1/2-\varepsilon} dE < \infty, \quad \forall \varepsilon > 0. \quad (9.10)$$

Equation (9.10) is proven, using (9.2), Theorem 9.7 in page 50 of [27] and Remark 9.9 in page 51 of [27].

To compute $\xi(E; H_{0,A,B}, H_0)$ we can use the diagonal representation with the matrices \tilde{A}, \tilde{B} in (3.25). Let us denote, respectively, by $-\Delta_D, -\Delta_N, -\Delta_\gamma$ the selfadjoint realizations of $-\frac{d^2}{dx^2}$ in $L^2((0, \infty), \mathbf{C})$ with Dirichlet boundary condition, $\varphi(0) = 0$, Neumann boundary condition, $\varphi'(0) = 0$ and with mixed boundary condition, $\varphi'(0) = \gamma\varphi(0)$.

With the notation of (3.26) we designate,

$$\gamma_j = -\cot \theta_j, \forall \theta_j \neq \pi, \pi/2. \quad (9.11)$$

Then,

$$\xi(E; H_{0,A,B}, H_0) = n_D \xi(E; -\Delta_D, -\Delta_N) + \sum_{j=1}^n \xi(E; -\Delta_{\gamma_j}, -\Delta_N), \quad (9.12)$$

where by $\sum_{j=1}^n$ we denote the sum over all $1 \leq j \leq n$ with $\theta_j \neq \pi, \pi/2$. Note that $\xi(E; -\Delta_N, -\Delta_N) = 0$. The spectral shift functions, $\xi(E; -\Delta_D, -\Delta_N), \xi(E; -\Delta_\gamma, -\Delta_N)$ can be easily computed as in Section 7 of Chapter 4 of [27] where $\xi(E; -\Delta_\gamma, -\Delta_D)$ is calculated. Observe that, $\xi(E; -\Delta_D, -\Delta_N) = -\xi(E; -\Delta_N, -\Delta_D)$. The result is as follows,

$$\xi(E; -\Delta_D, -\Delta_N) = \frac{1}{2}, \quad (9.13)$$

$$\xi(E; -\Delta_\gamma, -\Delta_N) = \frac{1}{2} - \frac{1}{\pi} \arctan\left(\frac{\sqrt{E}}{\gamma}\right), \quad \text{if } \gamma > 0, \quad (9.14)$$

$$\xi(E; -\Delta_\gamma, -\Delta_N) = -\frac{1}{2} - \frac{1}{\pi} \arctan\left(\frac{\sqrt{E}}{\gamma}\right), \quad \text{if } \gamma < 0. \quad (9.15)$$

Actually, (9.14), (9.15) follow from the computation in Section 7 of Chapter 4 of [27] since by the addition formula (Proposition 5 in page 275 of [26]), $\xi(E; -\Delta_\gamma, -\Delta_N) = \xi(E; -\Delta_\gamma, -\Delta_D) + \xi(E; -\Delta_D, -\Delta_N)$.

By (9.12), (9.13), (9.14), (9.15) it follows that,

$$\lim_{E \rightarrow \infty} \xi(E; H_{0,A,B}, H_0) = \frac{1}{2} n_D. \quad (9.16)$$

By (3.34), (3.35), (3.37)

$$\det S_{A,B}(k) = \det S_{A,B}(\infty) + O(1/|k|) \text{ as } k \rightarrow \infty, \quad (9.17)$$

where

$$\det S_{A,B}(\infty) = (-1)^{n_D}. \quad (9.18)$$

Then,

$$\lim_{k \rightarrow \infty} \arg [\det S_{A,B}(k)] = \begin{cases} 0 + 2\pi j, j = 0, \pm 1, \pm 2, \dots, & \text{if } n_D \text{ is even,} \\ \pi + 2\pi j, j = 0, \pm 1, \pm 2, \dots, & \text{if } n_D \text{ is odd.} \end{cases} \quad (9.19)$$

By the Birman-Krein formula (see equation (9.10) in page 47 of [27])

$$\det S(\sqrt{E}) = e^{-2\pi i \xi(E; H_{A,B}, H_0)}, \quad E > 0. \quad (9.20)$$

By (9.20), $-2\pi \xi(E; H_{A,B}, H_0)$ coincides, for $E > 0$, with one of the continuous branches of $\det S(\sqrt{E})$. By (9.19) this implies that $\lim_{k \rightarrow \infty} \xi(E; H_{A,B}, H_0)$ exists, and by (9.9), (9.16), also $\lim_{k \rightarrow \infty} \xi(E; H_{A,B}, H_{0,A,B})$ exists, but then, by (9.10),

$$\lim_{k \rightarrow \infty} \xi(E; H_{A,B}, H_{0,A,B}) = 0. \quad (9.21)$$

Hence, by (9.9), (9.16). (9.21)

$$\lim_{k \rightarrow \infty} \xi(E; H_{A,B}, H_0) = \frac{1}{2} n_D. \quad (9.22)$$

. Let us denote by $\Theta(k)$ the continuous branch of $\arg [\det S(k)]$ such that,

$$\lim_{k \rightarrow \infty} \Theta(k) = -\pi n_D. \quad (9.23)$$

If n_D is even this corresponds to $j = -n_D/2$ in (9.19) and to $j = -(n_D + 1)/2$ if n_D is odd. Then, by (9.20), (9.22) and (9.23) we have that,

$$\xi(E; H_{A,B}, H_0) = -\frac{1}{2\pi} \Theta(\sqrt{E}), \quad E > 0. \quad (9.24)$$

By (9.17), (9.22), (9.23) and (9.24),

$$\xi(E; H_{A,B}, H_0) = \frac{n_D}{2} + O\left(\frac{1}{\sqrt{E}}\right), \quad E \rightarrow \infty. \quad (9.25)$$

By (9.25)

$$\begin{cases} \int_{-\infty}^{\infty} |\xi(E; H_{A,B}, H_0)| (1 + |E|)^{-1-\varepsilon} dE < \infty, & \forall \varepsilon > 0, \text{ if } n_D > 0, \\ \int_{-\infty}^{\infty} |\xi(E; H_{A,B}, H_0)| (1 + |E|)^{-1/2-\varepsilon} dE < \infty, & \forall \varepsilon > 0, \text{ if } n_D = 0. \end{cases} \quad (9.26)$$

Let us denote by $\{E_j\}_{j=1}^P$ the eigenvalues of $H_{A,B}$ in increasing order $E_1 < E_2 < \dots < E_j < \dots$, with P finite or infinite. Let m_j be the multiplicity of E_j . Then by Proposition 9.2 in page 46 of [27] for $E < 0$, $\xi(E; H_{A,B}, H_0)$ is piecewise constant and it assumes integral values. Furthermore,

$$\xi(E; H_{A,B}, H_0) = 0, \text{ for } E < E_1, \quad (9.27)$$

$$\xi(E; H_{A,B}, H_0) = -m_1, \text{ for } E_1 < E < E_2, \dots, \xi(E; H_{A,B}, H_0) = -\sum_{j=1}^l m_j \text{ for } E_l < E < E_{l+1}. \quad (9.28)$$

Furthermore, by (9.26), (9.27) and (9.28)

$$\sum_{j=1}^{P-1} m_j (E_{j+1} - E_j) < \infty. \quad (9.29)$$

We summarize the results that we have obtained in the following theorem.

THEOREM 9.2. *Suppose that V satisfies (1.6), (1.7). Then, for $E < 0$, $\xi(E; H_{A,B}, H_0)$ is piecewise constant, it assumes integral values, and (9.27), (9.28) and (9.29) hold. For $E > 0$ (9.24) is valid, where $\Theta(k)$ is the continuous branch of $\arg[\det S(\sqrt{E})]$ that satisfies (9.23). Moreover, (9.25) and (9.26) are true. Suppose that the function f has two locally bounded derivatives and that for some $\varepsilon > 0$,*

$$f'(E) = O\left(\frac{1}{E^{1+\varepsilon}}\right), f''(E) = O\left(\frac{1}{E^{2+\varepsilon}}\right), \quad \text{as } E \rightarrow \infty. \quad (9.30)$$

Then $f(H_{A,B}) - f(H_0)$ is trace class and

$$\text{Tr}(f(H_{A,B}) - f(H_0)) = \int_{-\infty}^{\infty} \xi(E; H_{A,B}, H_0) f'(E) dE. \quad (9.31)$$

Proof: it only remains to prove (9.31). However, this formula follows from (9.9) and applying Theorem 9.7 in page 50 of [27] and Remark 9.9 in page 51 of [27] to $f(H_{0,A,B}) - f(H_0)$ and to $f(H_{A,B}) - f(H_{0,A,B})$ using, respectively, (9.1) and (9.2).

If V satisfies,

$$\int_0^{\infty} dx (1+x) \|V(x)\| < +\infty, \quad (9.32)$$

the total number of bound states, including multiplicity, \mathcal{N} , is finite (see Theorems 8.1 and 8.6 of [7]). Then, by (9.28)

$$\xi(0-; H_{A,B}, H_0) =: \lim_{E \uparrow 0} \xi(E; H_{A,B}, H_0) = -\mathcal{N}. \quad (9.33)$$

In the following theorem we give a Levinson's theorem for the spectral shift function.

THEOREM 9.3. *Suppose that V satisfies (1.7), (9.32), and let $\mathcal{N} < \infty$ be the number of bound states of $H_{A,B}$ including multiplicities. Then, denoting $\xi(0+; H_{A,B}, H_0) := \lim_{E \downarrow 0} \xi(E; H_{A,B}, H_0)$,*

$$\xi(0+, H_{A,B}, H_0) = \frac{1}{2} [n - \mu] - \mathcal{N}, \quad (9.34)$$

where μ is the (algebraic and geometric) multiplicity of the eigenvalue $+1$ of the zero-energy scattering matrix $S_{A,B}(0)$.

Proof: Equation (9.29) follows from equation (9.13) of [7], (9.23) and (9.24).

References

- [1] V. Kostykin and R. Schrader, *Kirchhoff's rule for quantum wires*, J. Phys. A **32**, 595–630 (1999).
- [2] V. Kostykin and R. Schrader, *Kirchhoff's rule for quantum wires. II: The inverse problem with possible applications to quantum computers*, Fortschr. Phys. **48**, 703–716 (2000).
- [3] M. S. Harmer, *Inverse scattering for the matrix Schrödinger operator and Schrödinger operator on graphs with general self-adjoint boundary conditions*, ANZIAM J. **44**, 161–168 (2002).
- [4] M. S. Harmer, *The matrix Schrödinger Operator and Schrödinger Operator on Graphs*, Ph.D. thesis, University of Auckland, New Zealand, 2004.
- [5] M. S. Harmer, *Inverse scattering on matrices with boundary conditions*, J. Phys. A **38**, 4875–4885 (2005).
- [6] T. Aktosun, M. Klaus, and R. Weder, *Small-energy analysis for the self-adjoint matrix Schrödinger equation on the half line*, J. Math. Phys. **52**, 102101 (2011).
- [7] T. Aktosun, and R. Weder, *High-energy analysis and Levinson's theorem for the self-adjoint matrix Schrödinger operator on the half line*, J. Math. Phys. **54**, 012108 (2013).
- [8] T. Aktosun, M. Klaus, and R. Weder, *Small-energy analysis for the self-adjoint matrix Schrödinger operator on the half line II*, J. Math. Phys. **55**, 032103 (2014).
- [9] N. I. Gerasimenko, *The inverse scattering problem on a noncompact graph*, Theoret. Math. Phys. **75**, 460–470 (1988).
- [10] N. I. Gerasimenko and B. S. Pavlov, *A scattering problem on noncompact graphs*, Theoret. Math. Phys. **74**, 230–240 (1988).
- [11] B. Gutkin and U. Smilansky, *Can one hear the shape of a graph?* J. Phys. A **34**, 6061–6068 (2001).
- [12] P. Kurasov and F. Stenberg, *On the inverse scattering problem on branching graphs*, J. Phys. A **35**, 101–121 (2002).
- [13] P. Kuchment, *Quantum graphs. I. Some basic structures*, Waves Random Media **14**, S107–S128 (2004).
- [14] J. Boman and P. Kurasov, *Symmetries of quantum graphs and the inverse scattering problem*, Adv. Appl. Math. **35**, 58–70 (2005).
- [15] P. Kuchment, *Quantum graphs. II. Some spectral properties of quantum and combinatorial graphs*, J. Phys. A **38**, 4887–4900 (2005).

- [16] P. Kurasov and M. Nowaczyk, *Inverse spectral problem for quantum graphs*, J. Phys. A **38**, 4901–4915 (2005).
- [17] G. Berkolaiko, R. Carlson, S. A. Fulling, and P. Kuchment (eds.), *Quantum Graphs and their Applications*, Contemporary Mathematics, 415, Amer. Math. Soc., Providence, RI, 2006.
- [18] P. Exner, J. P. Keating, P. Kuchment, T. Sunada, and A. Teplyaev (eds.), *Analysis on graphs and its applications*, Proc. Symposia in Pure Mathematics, 77, Amer. Math. Soc., Providence, RI, 2008.
- [19] J. Behrndt and A. Luger, *On the number of negative eigenvalues of the Laplacian on a metric graph*, J. Phys. A **43**, 474006 (2010).
- [20] P. Kurasov and M. Nowaczyk, *Geometric properties of quantum graphs and vertex scattering matrices*, Opuscula Mathematica **30**, 295–309 (2010).
- [21] G. Berkolaiko and P. Kuchment, *Introduction to Quantum Graphs*. Mathematical Surveys and Monographs **186** Am. Math. Soc, Providence, R I 2013.
- [22] Z. S. Agranovich and V. A. Marchenko, *The Inverse Problem of Scattering Theory*, Gordon and Breach, New York, 1963.
- [23] J. Behrndt, M. M. Malamud, and H. Neidhardt, *Scattering matrices and Weyl functions*, Proc. London Math. Soc. **97**, 568–598 (2008).
- [24] L. Hörmander, *The analysis of Linear Partial differential Operators II*, Springer-Verlag, Berlin, 1983.
- [25] R. Weder, *Spectral and Scattering Theory for Perturbed Stratified Media*, Applied Mathematical Sciences **87**, Springer-Verlag, New York, 1991.
- [26] D. R. Yafaev, *Mathematical Scattering Theory: General Theory*, Amer. Math. Soc. Providence, Rhode Island, 1992.
- [27] D. R. Yafaev, *Mathematical Scattering Theory: Analytic Theory*, Amer. Math. Soc. Providence, Rhode Island, 2010.
- [28] R. A. Adams, J. J. F. Fournier, *Sobolev Spaces*, Elsevier Science, Oxford, U.K., 2003.
- [29] V. A. Marchenko, *Sturm-Liouville Operators and Applications*, Birkhäuser, Basel, 1986.
- [30] B. M. Levitan, *Inverse Sturm-Liouville Problems*, VNU Science Press, Utrecht, 1987.
- [31] T. Aktosun and R. Weder, *Inverse spectral-scattering problem with two sets of discrete spectra for the radial Schrödinger equation*, Inverse Problems **22**, 89–114 (2006).
- [32] T. Kato, *Perturbation Theory of Linear Operators. Second Edition*, Springer, Berlin, 1976.